



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 03:07 PM UTC

PDB ID : 8U10 / pdb_00008u10
EMDB ID : EMD-41791
Title : In situ cryo-EM structure of bacteriophage P22 gp1:gp4:gp5:gp10:gp9 N-term complex in conformation 1 at 3.2Å resolution
Authors : Iglesias, S.; Feng-Hou, C.; Cingolani, G.
Deposited on : 2023-08-30
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

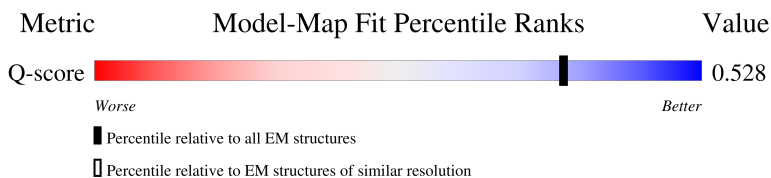
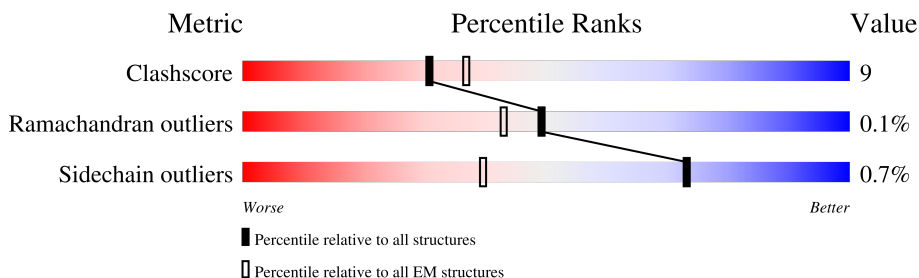
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	725	35% 59% 16% 25%
1	b	725	34% 60% 15% 25%
1	c	725	35% 61% 13% 25%
1	d	725	31% 61% 14% 25%

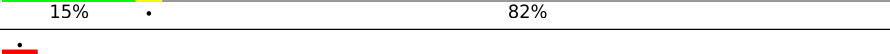
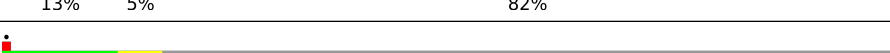
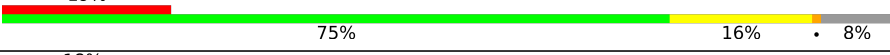
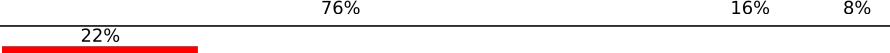
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Mol	Chain	Length	Quality of chain
1	e	725	
1	f	725	
1	g	725	
1	h	725	
1	i	725	
1	j	725	
1	k	725	
1	l	725	
2	A	430	
2	B	430	
2	C	430	
2	D	430	
2	E	430	
2	F	430	
2	G	430	
2	H	430	
2	I	430	
2	J	430	
3	1	472	
3	2	472	
3	3	472	
3	4	472	
3	5	472	
3	6	472	
4	10	667	

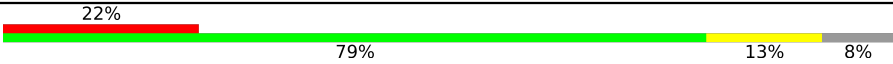
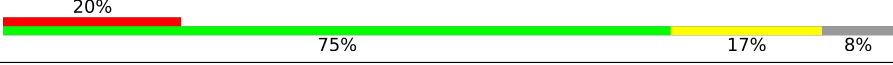
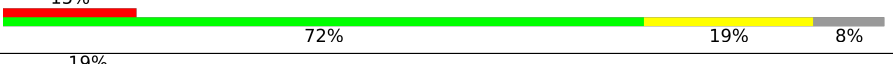
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Mol	Chain	Length	Quality of chain
4	11	667	
4	12	667	
4	13	667	
4	14	667	
4	15	667	
4	16	667	
4	17	667	
4	18	667	
4	19	667	
4	20	667	
4	21	667	
4	22	667	
4	23	667	
4	24	667	
4	7	667	
4	8	667	
4	9	667	
5	m	166	
5	n	166	
5	o	166	
5	p	166	
5	q	166	
5	r	166	
5	s	166	
5	t	166	

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Mol	Chain	Length	Quality of chain
5	u	166	
5	v	166	
5	x	166	
5	y	166	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138386 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	b	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	c	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	d	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	e	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	l	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	f	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	k	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	i	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	j	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	h	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
1	g	544	Total 4417	C 2791	N 756	O 850	S 20	0	0

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	429	Total 3277	C 2053	N 568	O 643	S 13	0	0
2	C	429	Total 3277	C 2053	N 568	O 643	S 13	0	0
2	A	429	Total 3277	C 2053	N 568	O 643	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
2	I	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
2	D	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
2	B	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
2	F	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
2	H	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
2	J	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		

- Molecule 3 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
3	2	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
3	3	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
3	4	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
3	5	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
3	6	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

- Molecule 4 is a protein called Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	16	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
4	17	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
4	18	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
4	22	120	Total	C	N	O	S	0	0
			934	595	156	182	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	23	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	24	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	19	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	20	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	21	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	10	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	11	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	12	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	13	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	14	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	15	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	7	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	8	120	Total 934	C 595	N 156	O 182	S 1	0	0
4	9	120	Total 934	C 595	N 156	O 182	S 1	0	0

- Molecule 5 is a protein called Peptidoglycan hydrolase gp4.

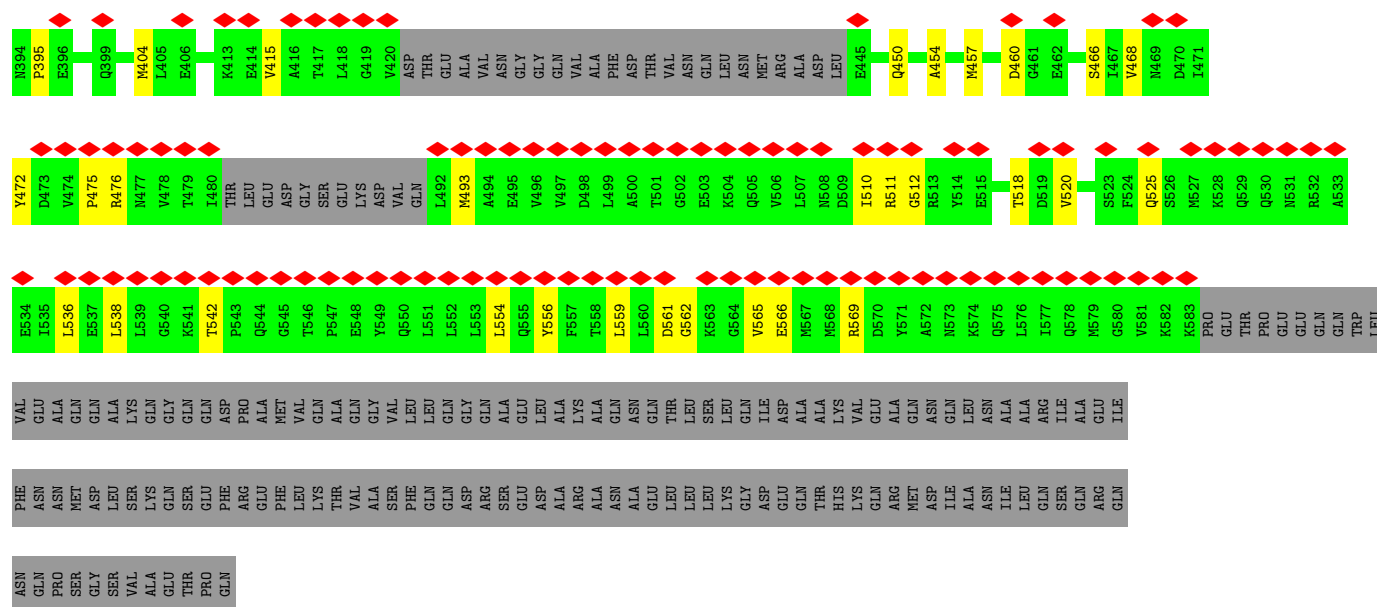
Mol	Chain	Residues	Atoms					AltConf	Trace
5	y	152	Total 1166	C 731	N 200	O 229	S 6	0	0
5	m	152	Total 1166	C 731	N 200	O 229	S 6	0	0
5	n	152	Total 1166	C 731	N 200	O 229	S 6	0	0
5	o	152	Total 1166	C 731	N 200	O 229	S 6	0	0
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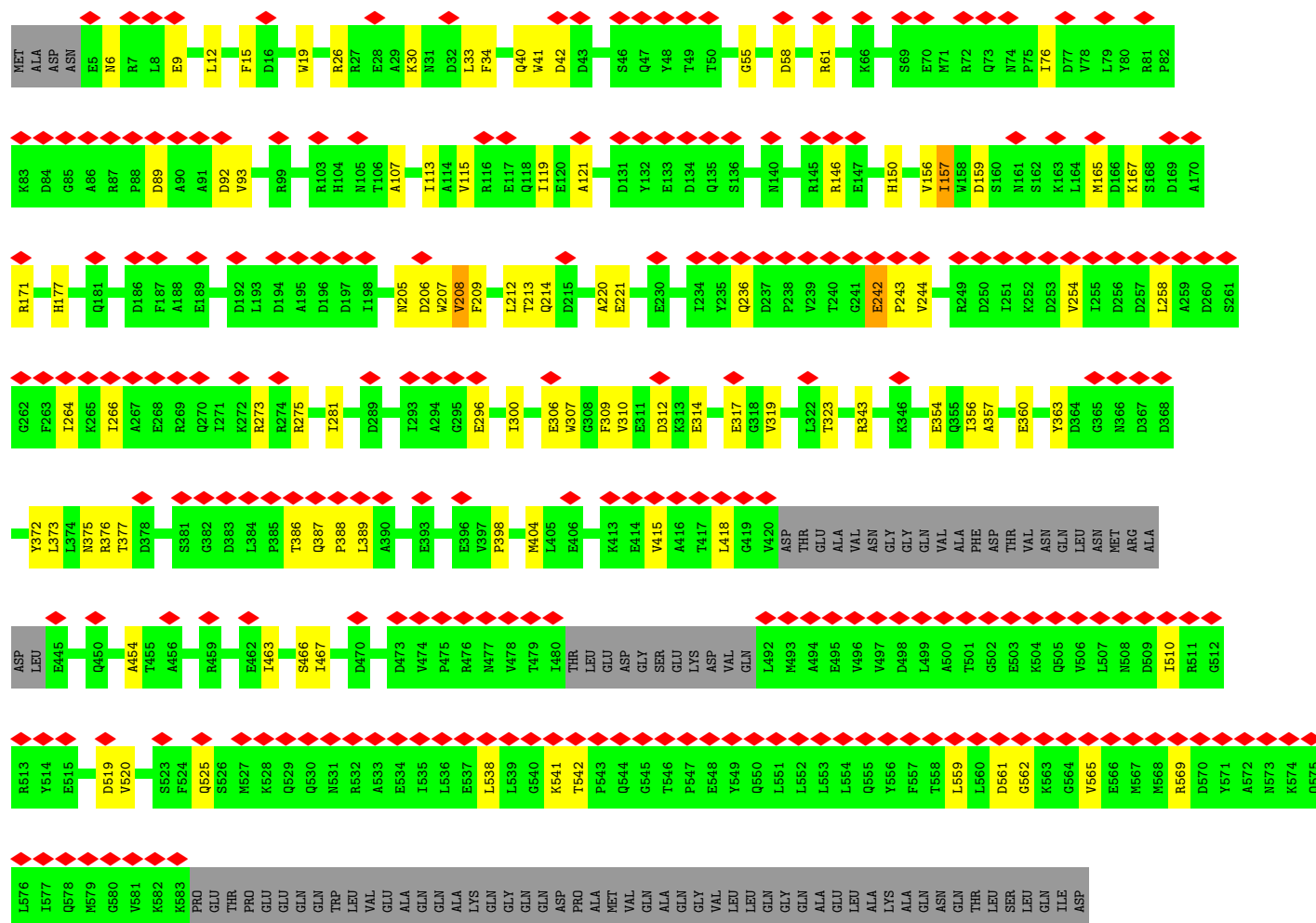
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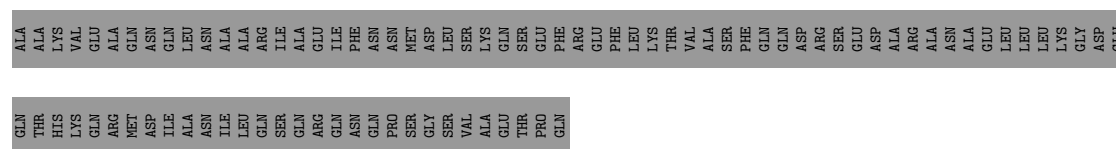
Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	r	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	s	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	t	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	u	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	v	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
5	x	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		

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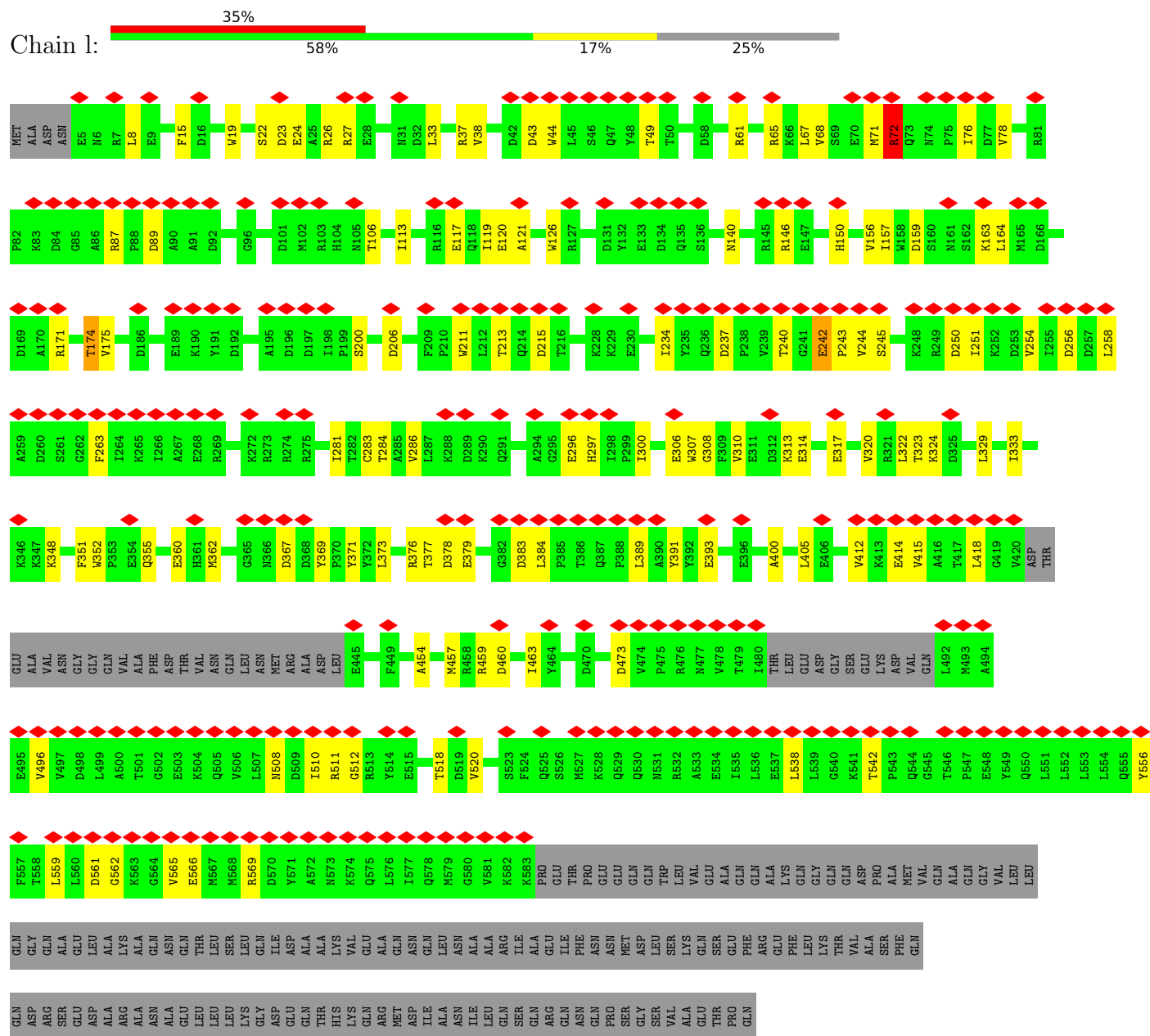


- Molecule 1: Portal protein

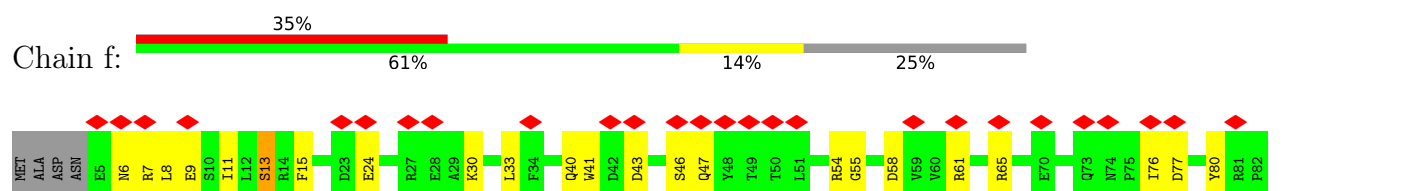




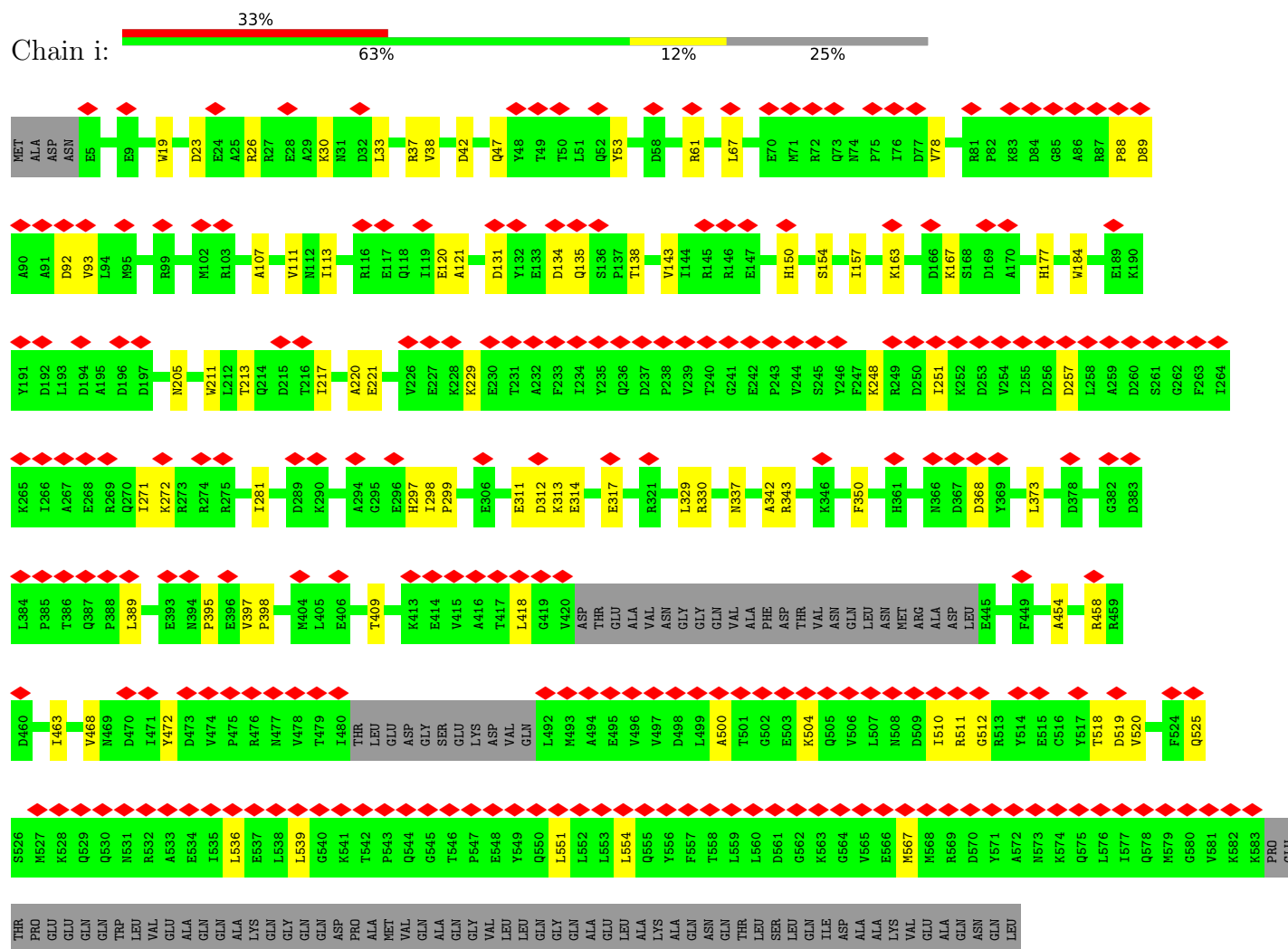
• Molecule 1: Portal protein

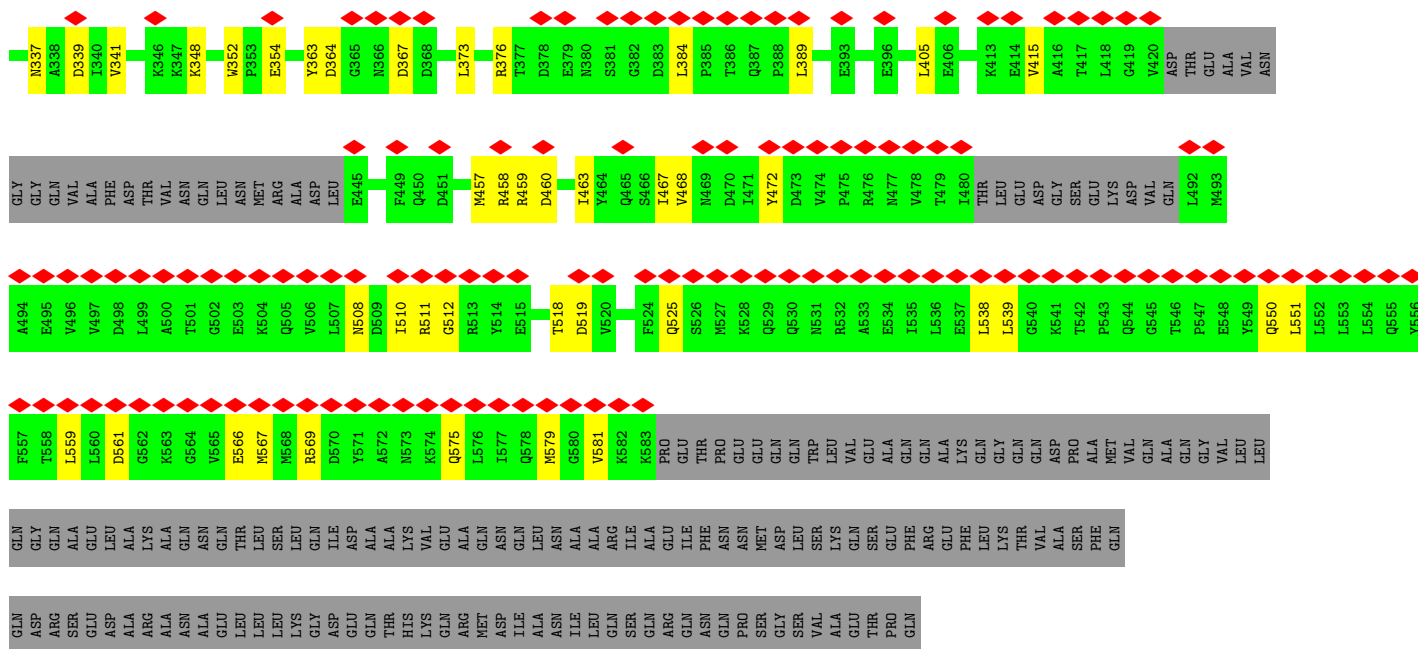


• Molecule 1: Portal protein

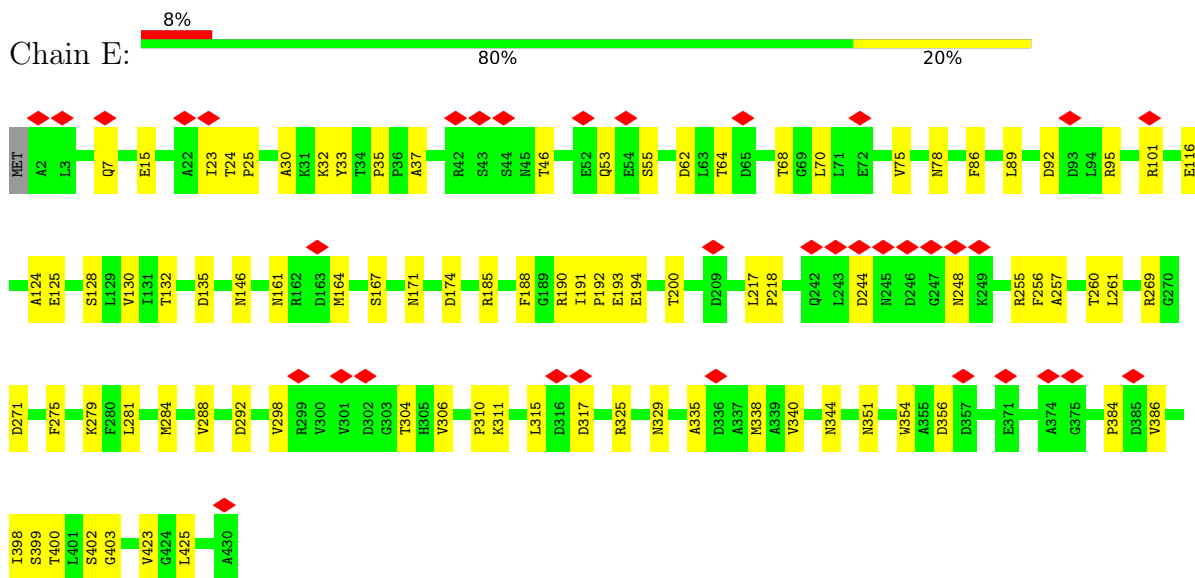


- Molecule 1: Portal protein

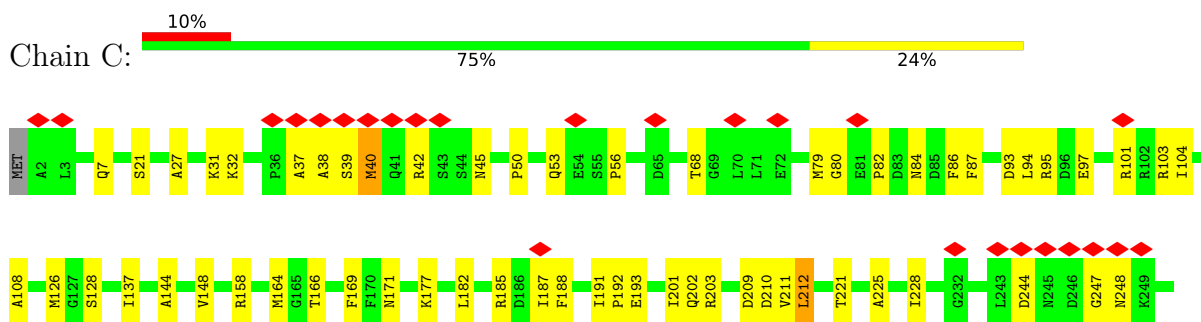


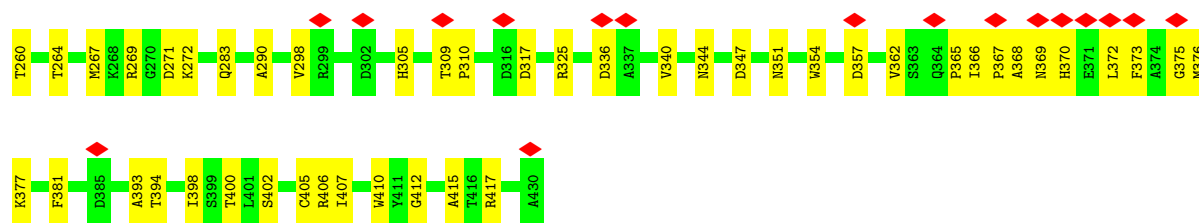


- Molecule 2: Major capsid protein

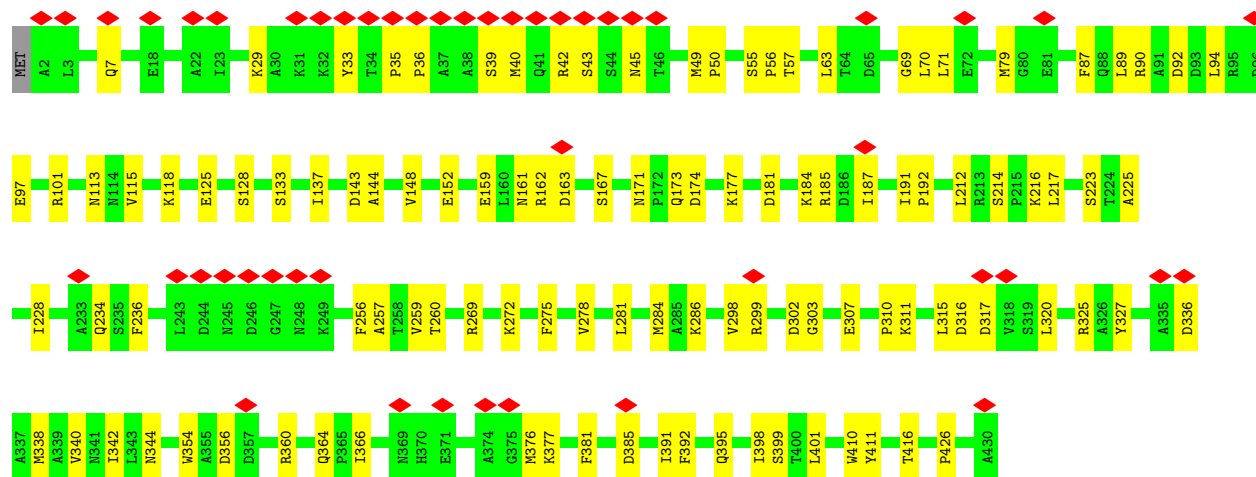
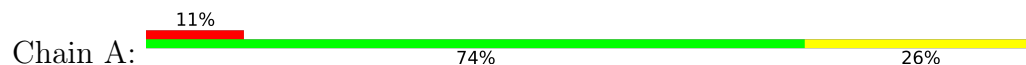


- Molecule 2: Major capsid protein

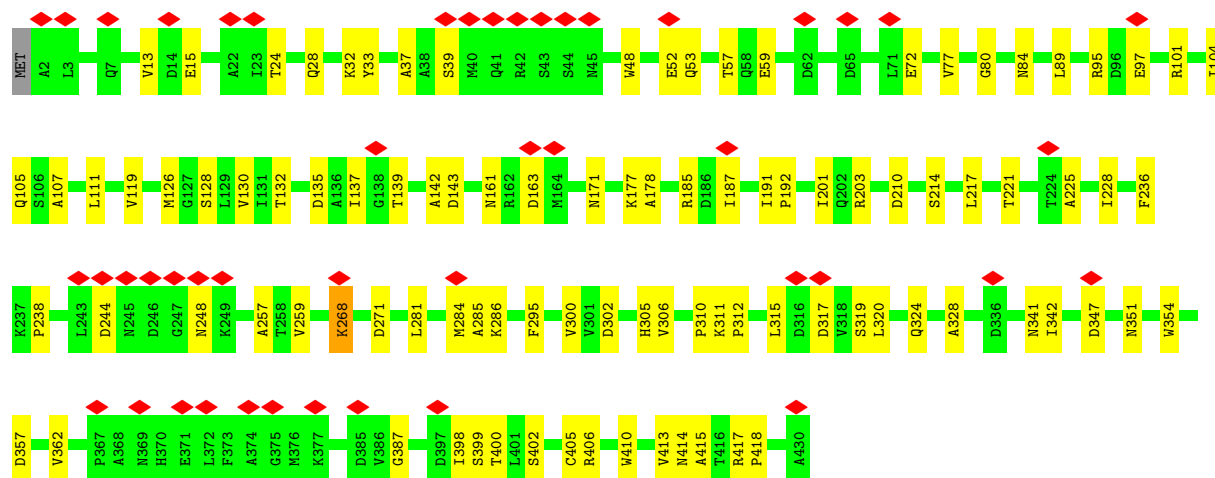




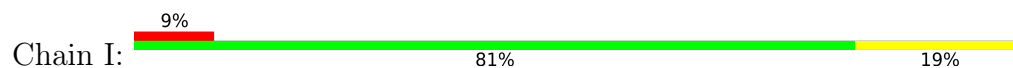
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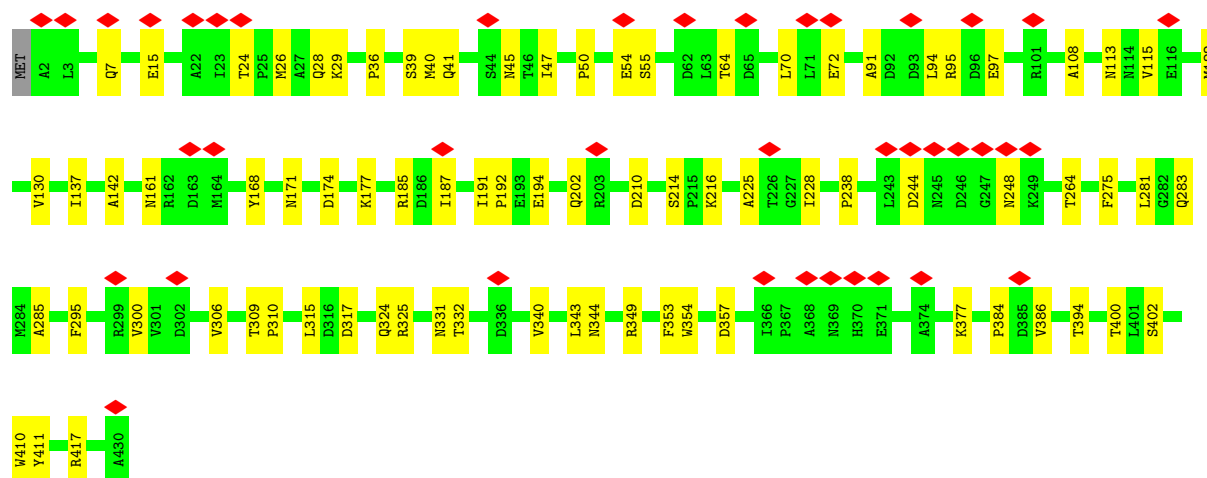


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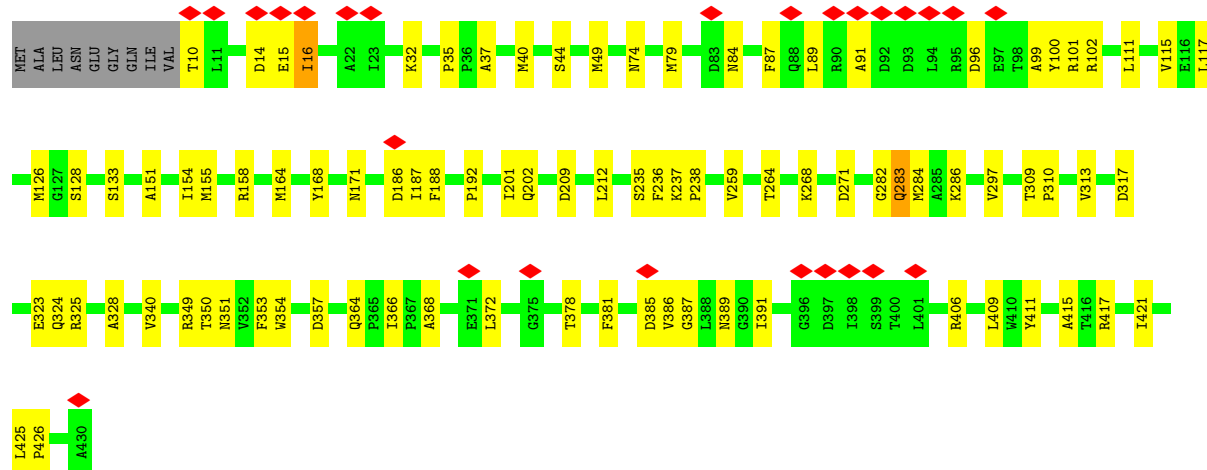
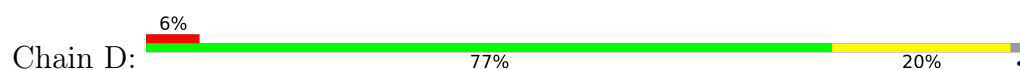


• Molecule 2: Major capsid protein

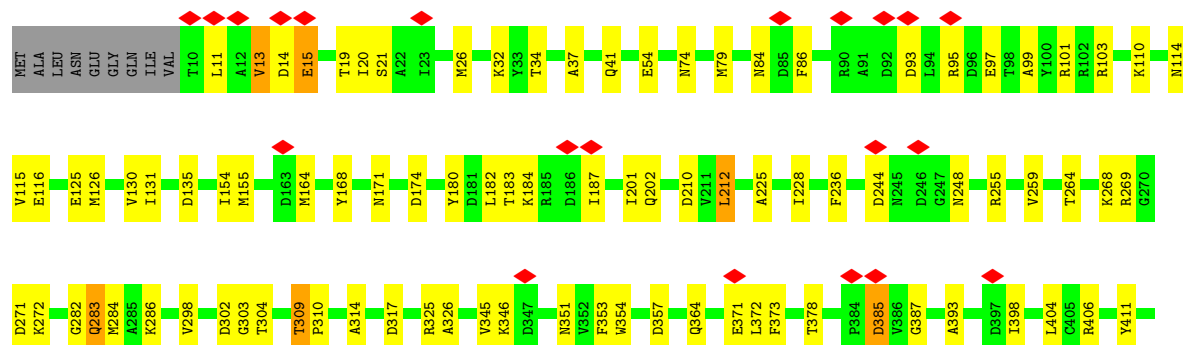
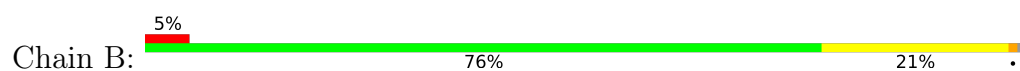




• Molecule 2: Major capsid protein

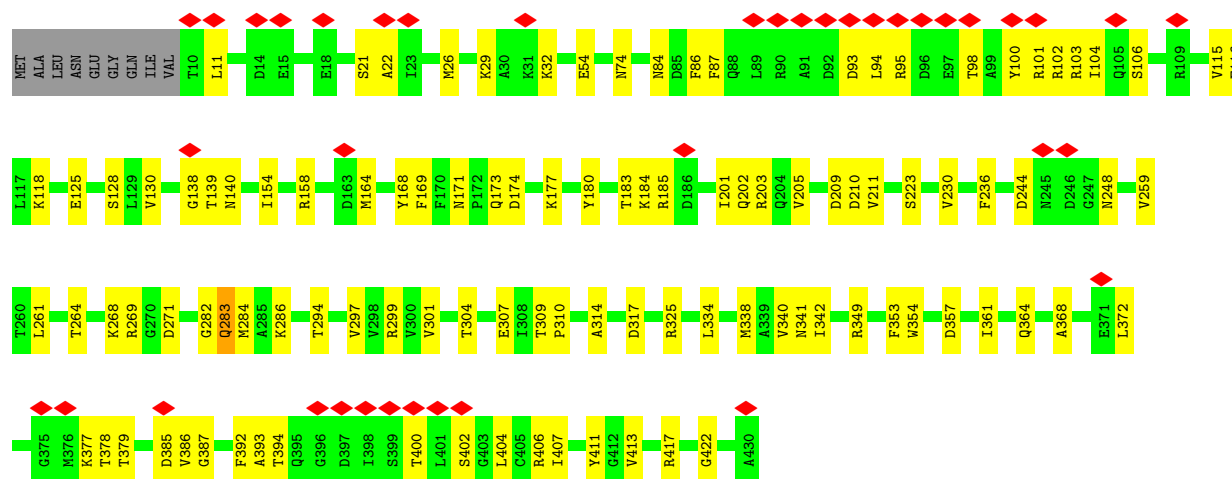


• Molecule 2: Major capsid protein

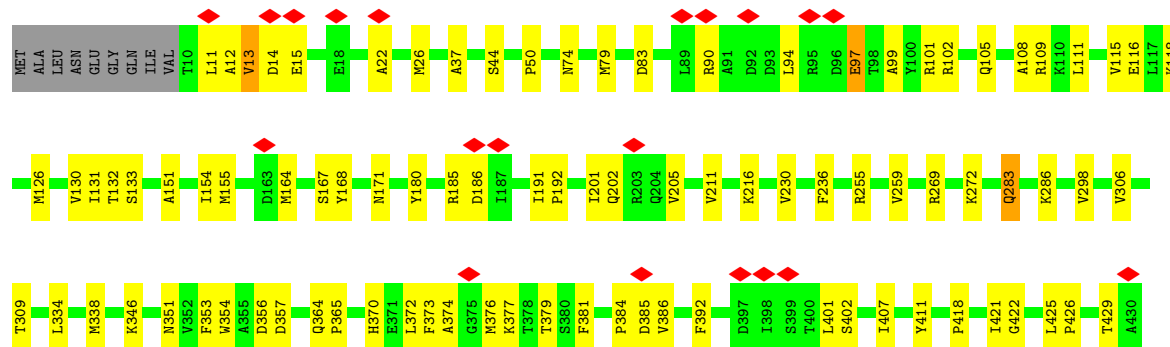
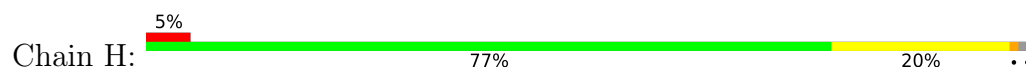




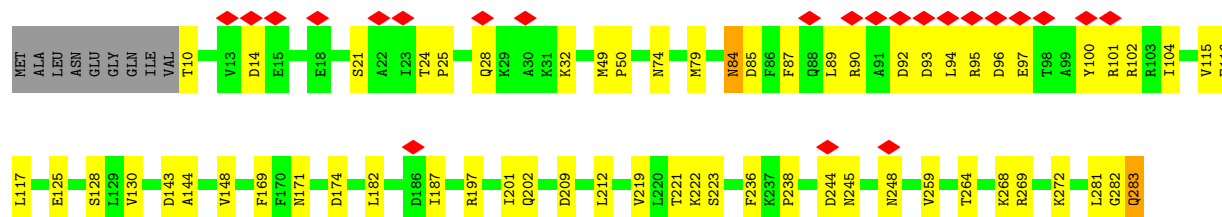
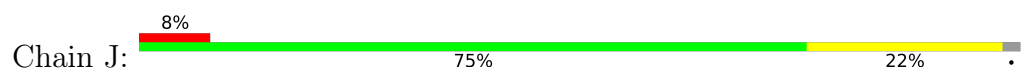
• Molecule 2: Major capsid protein

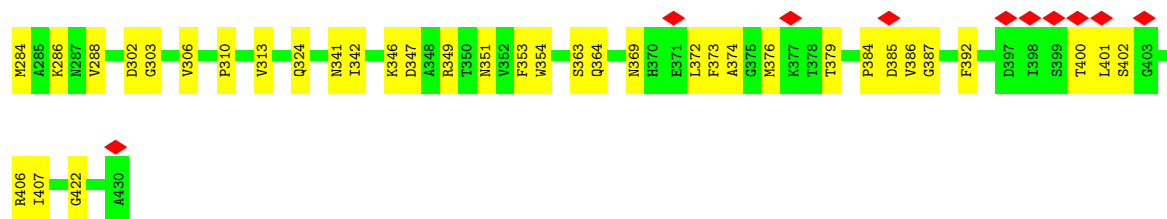


• Molecule 2: Major capsid protein

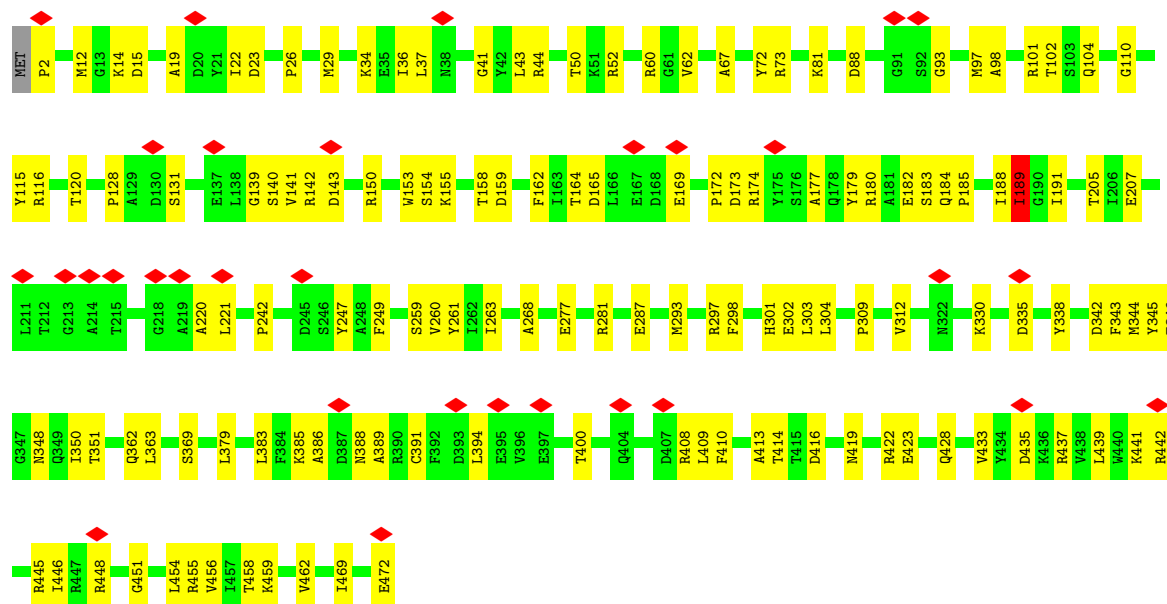
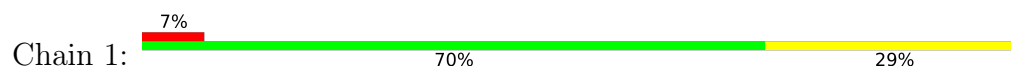


• Molecule 2: Major capsid protein

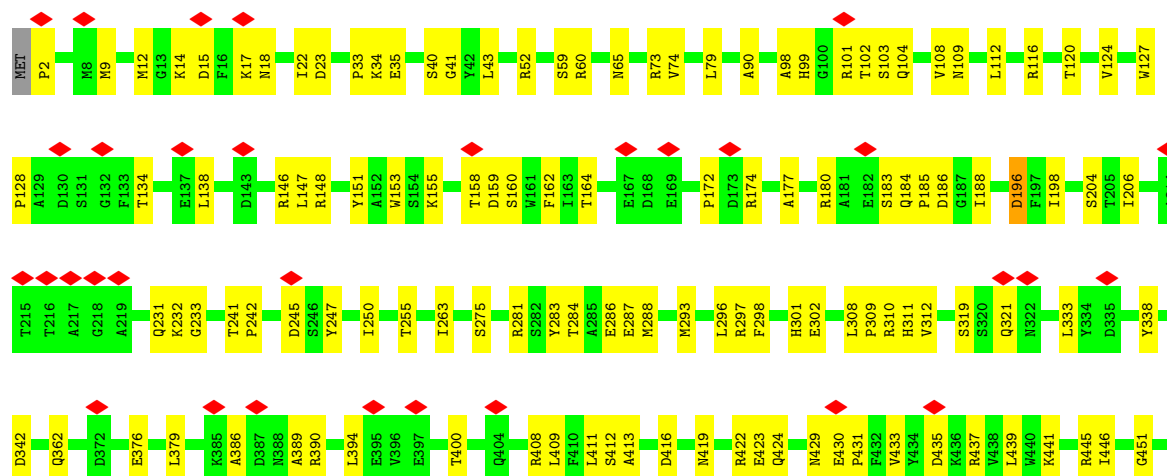
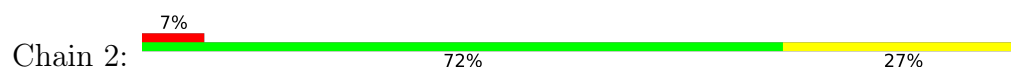


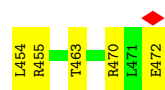


• Molecule 3: Packaged DNA stabilization protein gp10

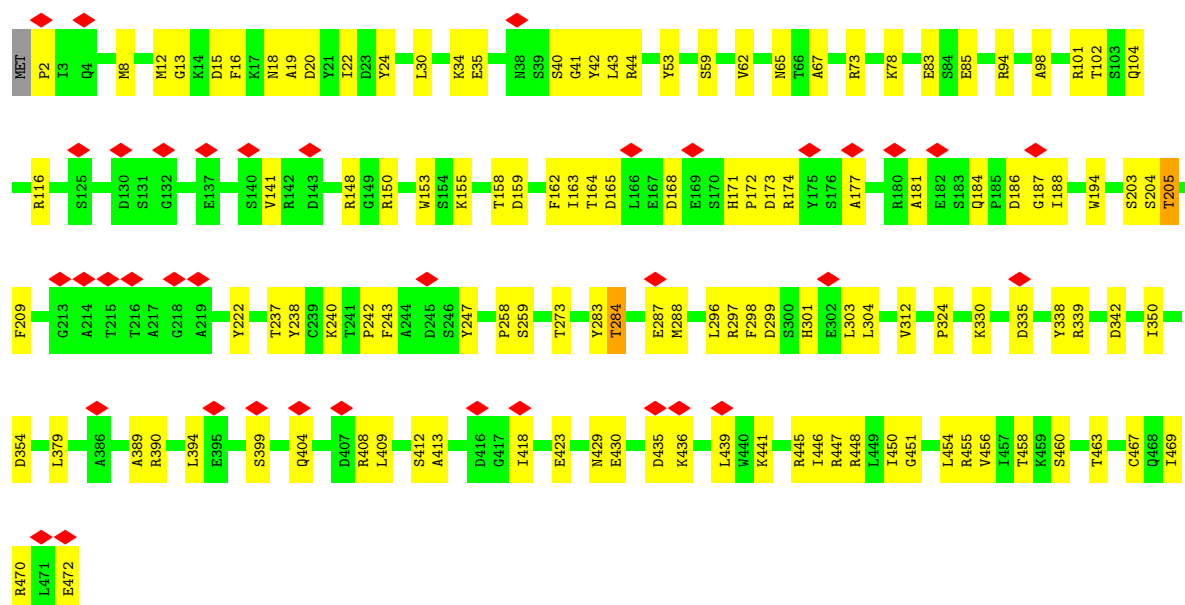
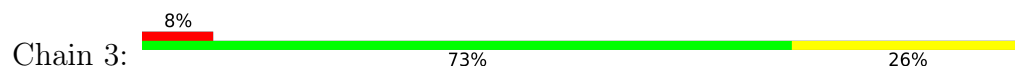


• Molecule 3: Packaged DNA stabilization protein gp10

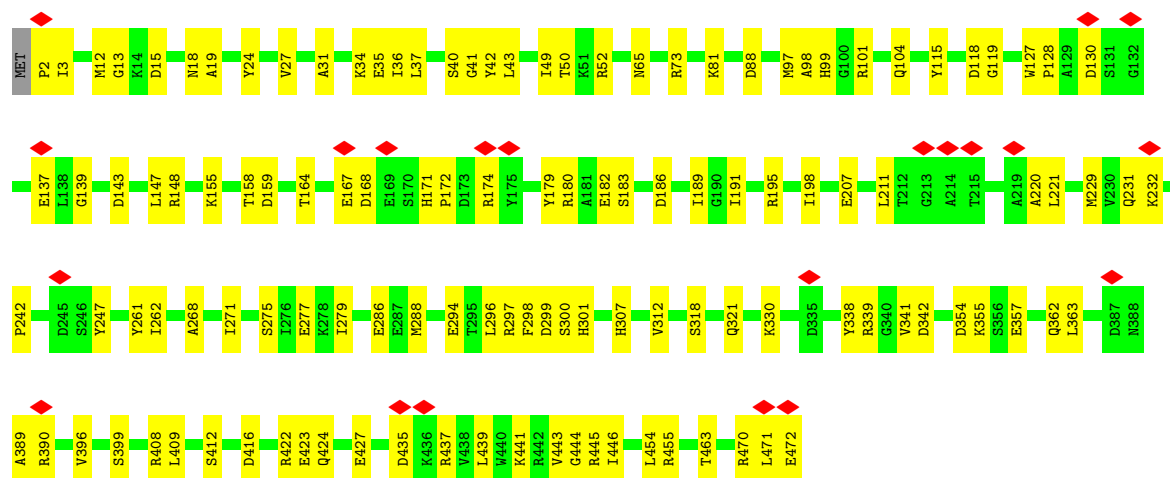




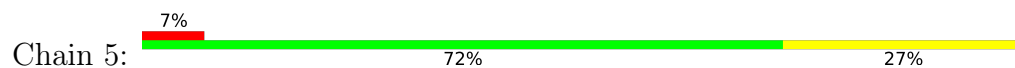
• Molecule 3: Packaged DNA stabilization protein gp10

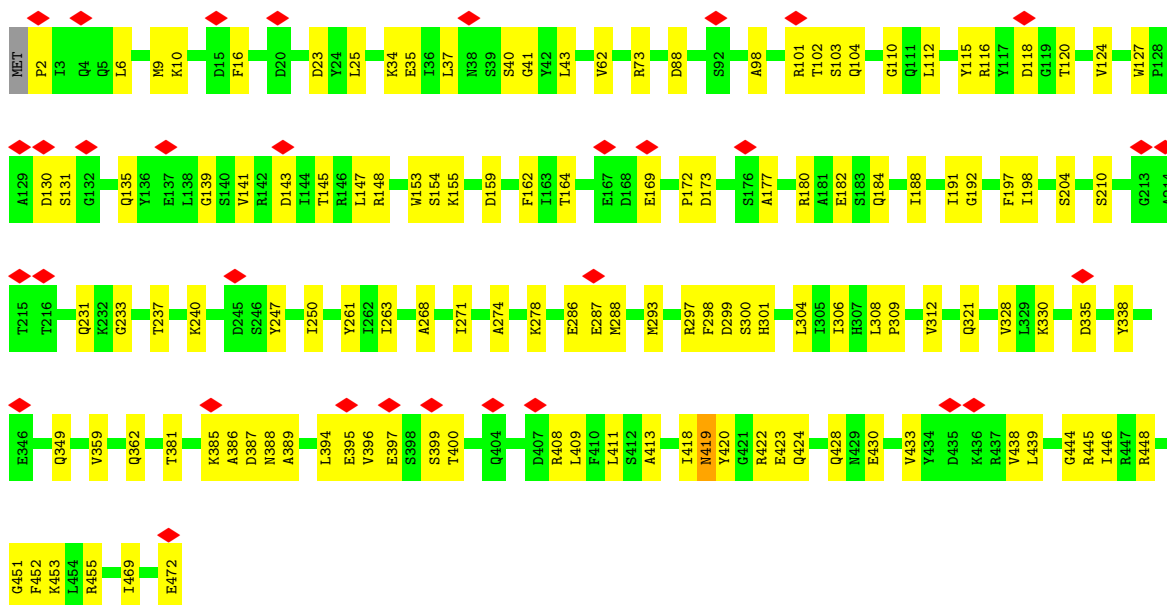


• Molecule 3: Packaged DNA stabilization protein gp10

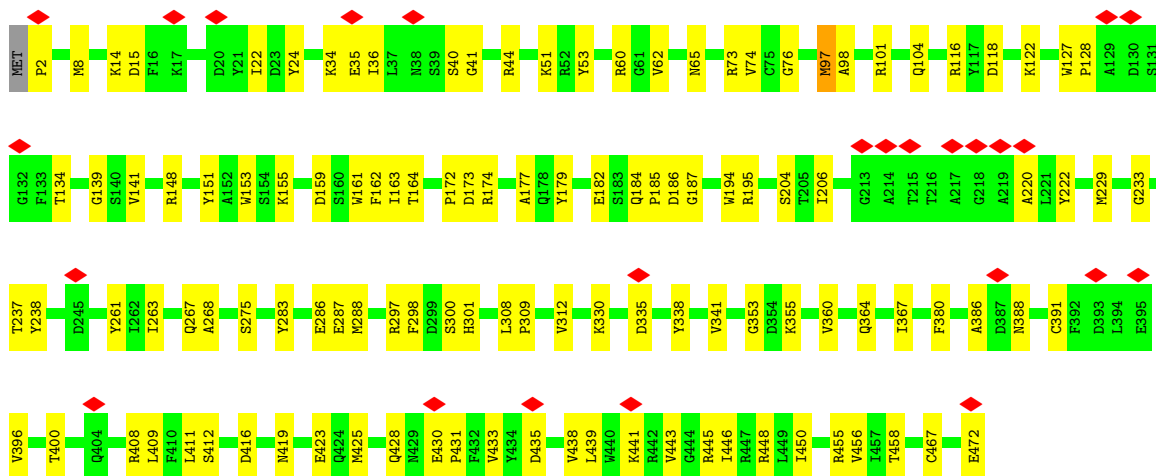
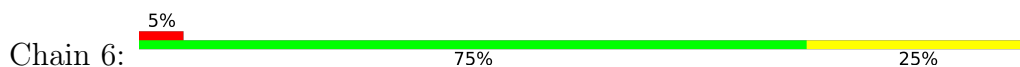


• Molecule 3: Packaged DNA stabilization protein gp10

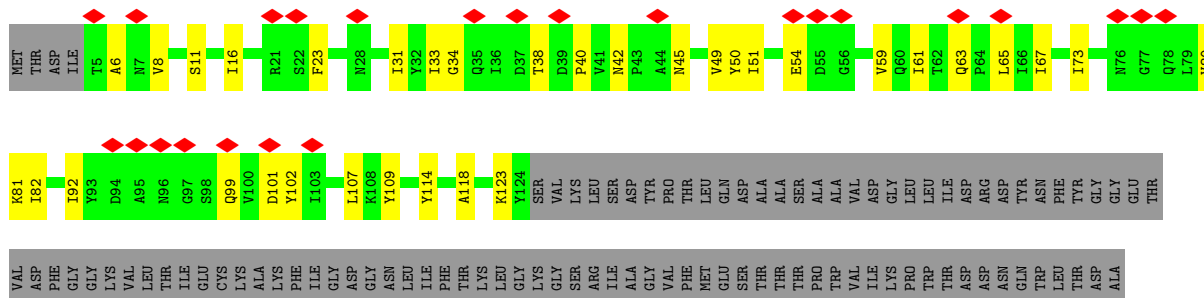




• Molecule 3: Packaged DNA stabilization protein gp10

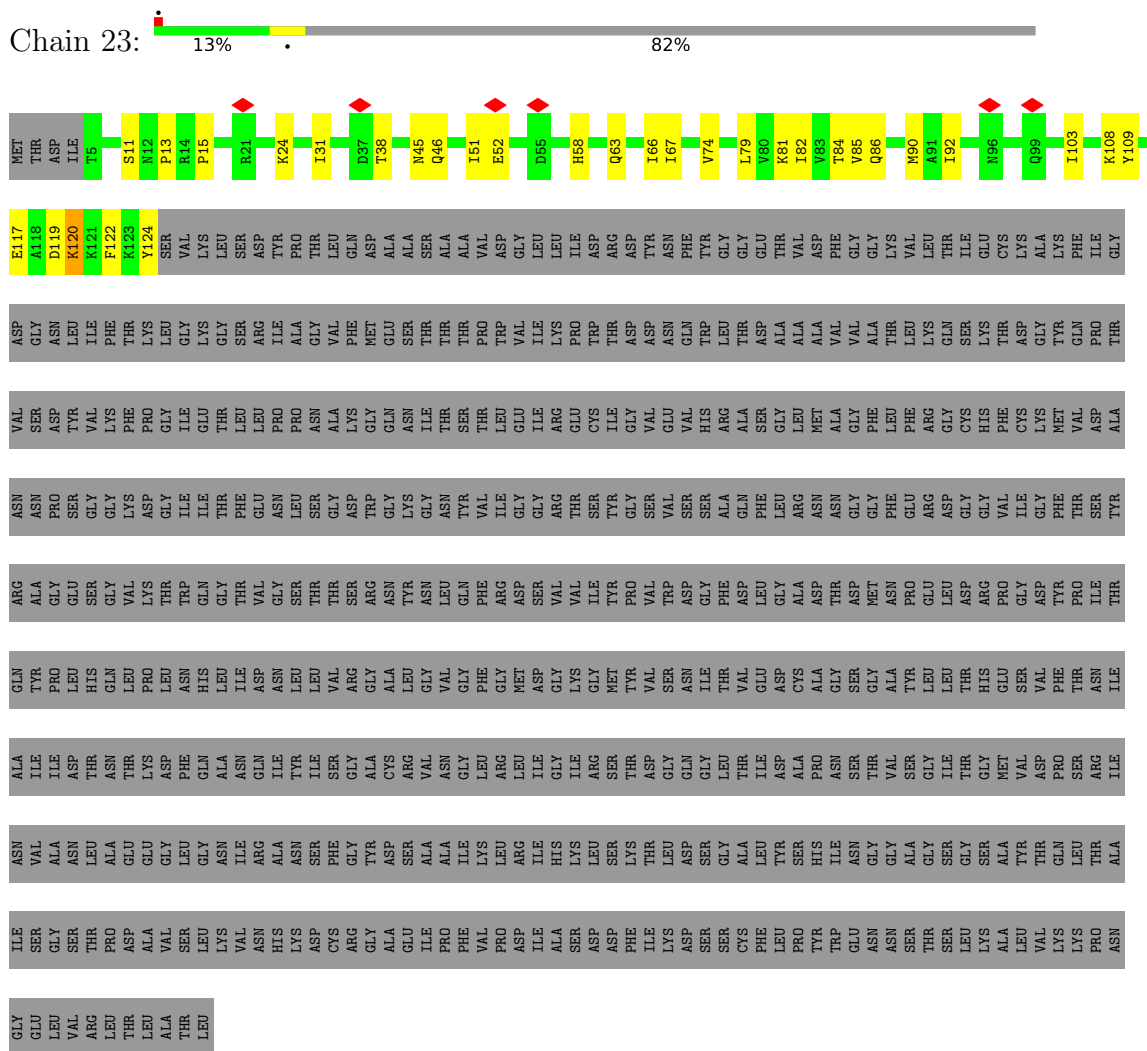


• Molecule 4: Tail spike protein



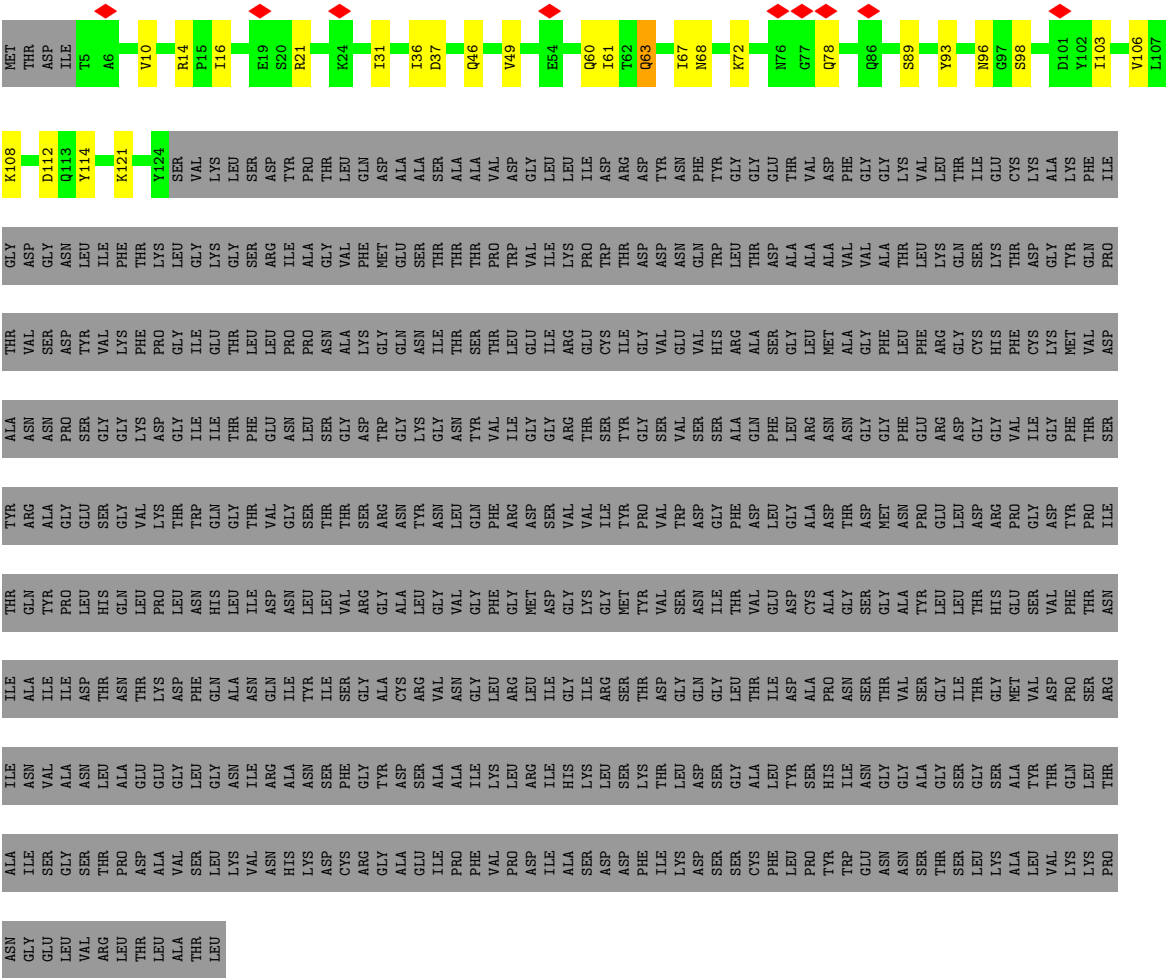
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- Molecule 4: Tail spike protein

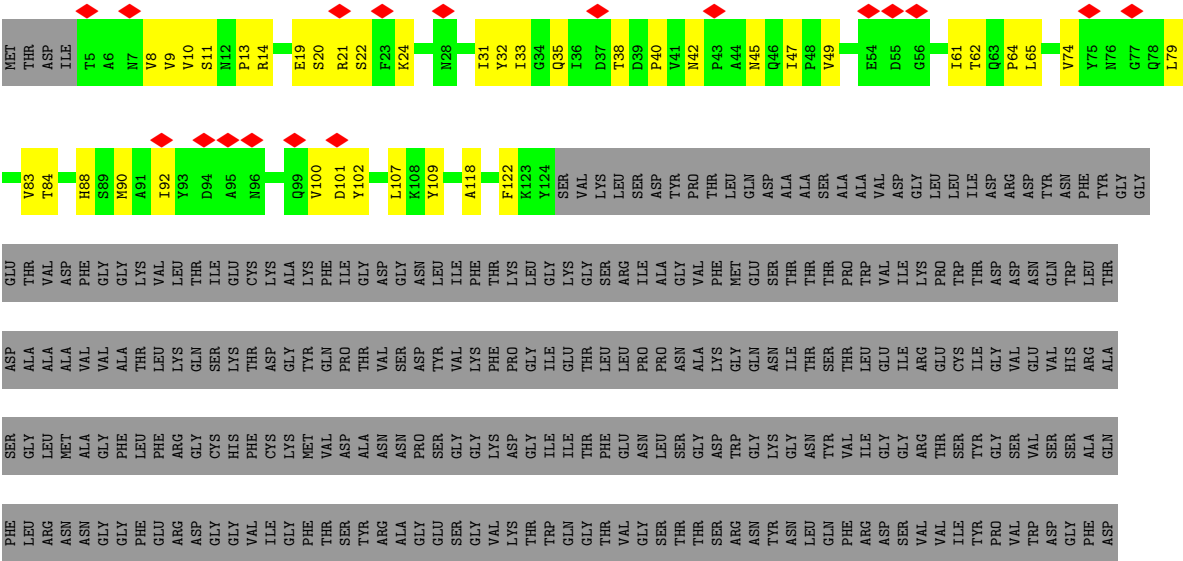


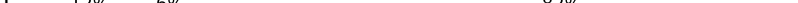
- Molecule 4: Tail spike protein

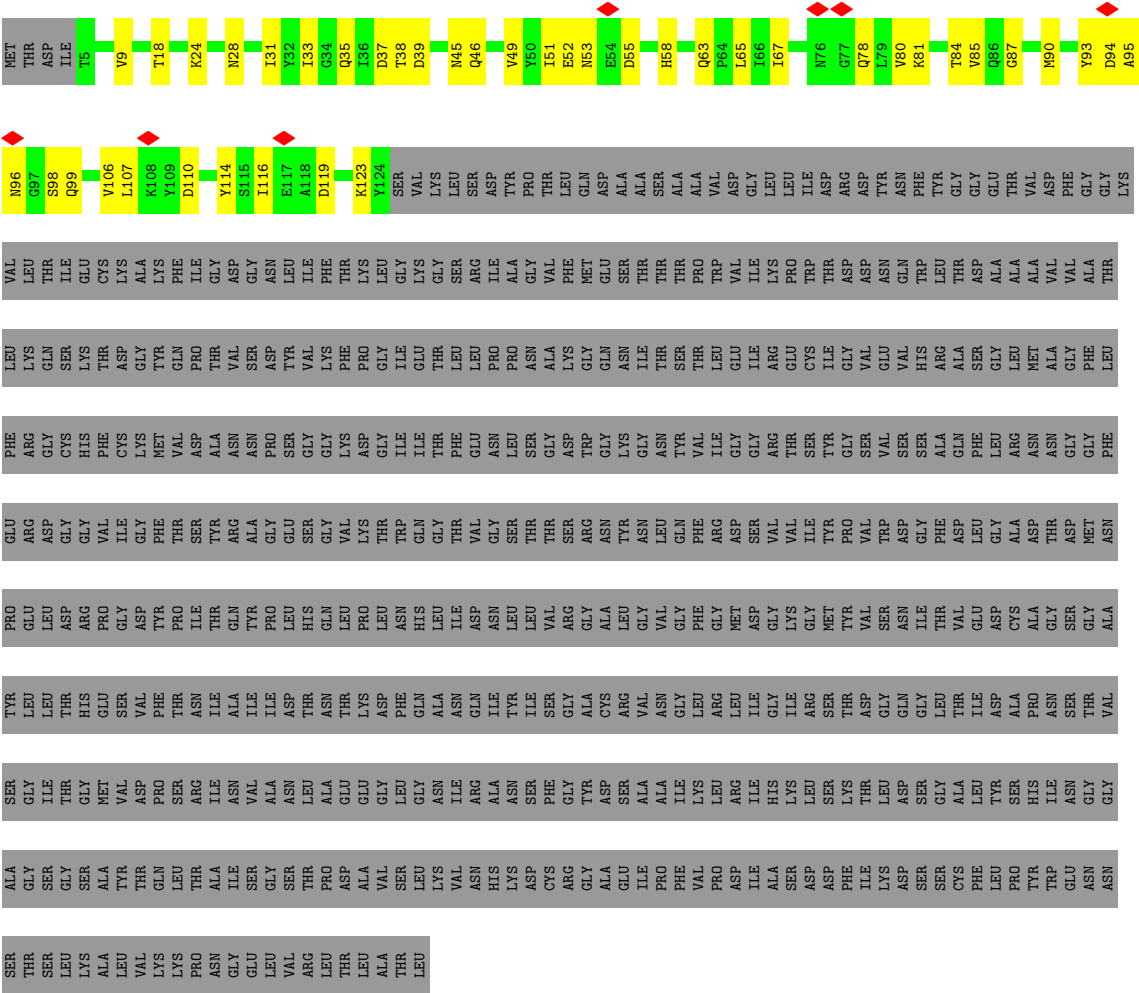




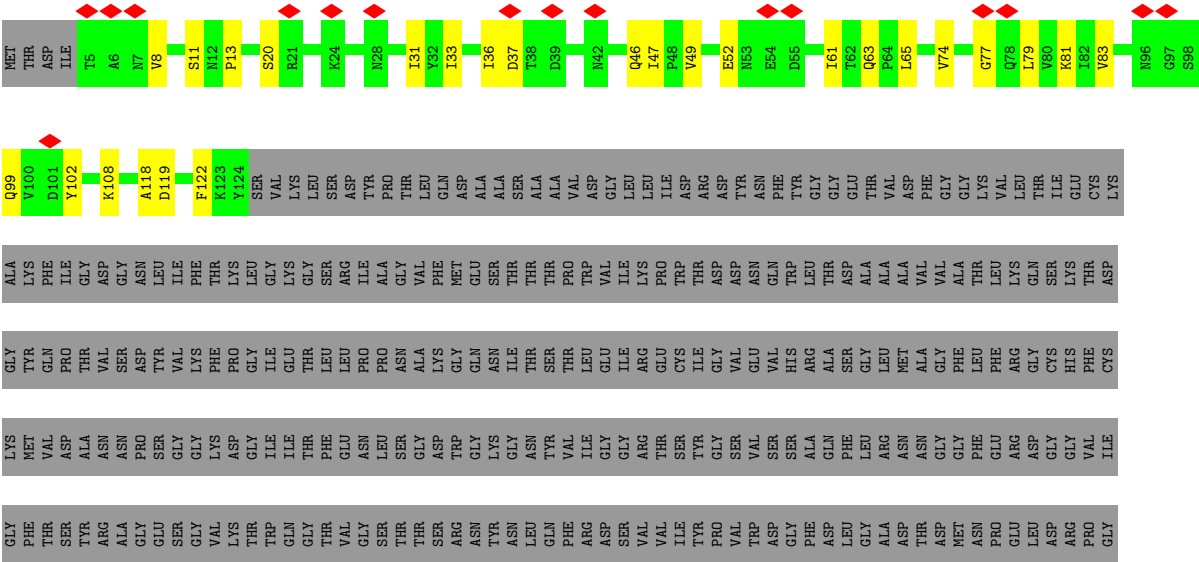
● Molecule 4: Tail spike protein



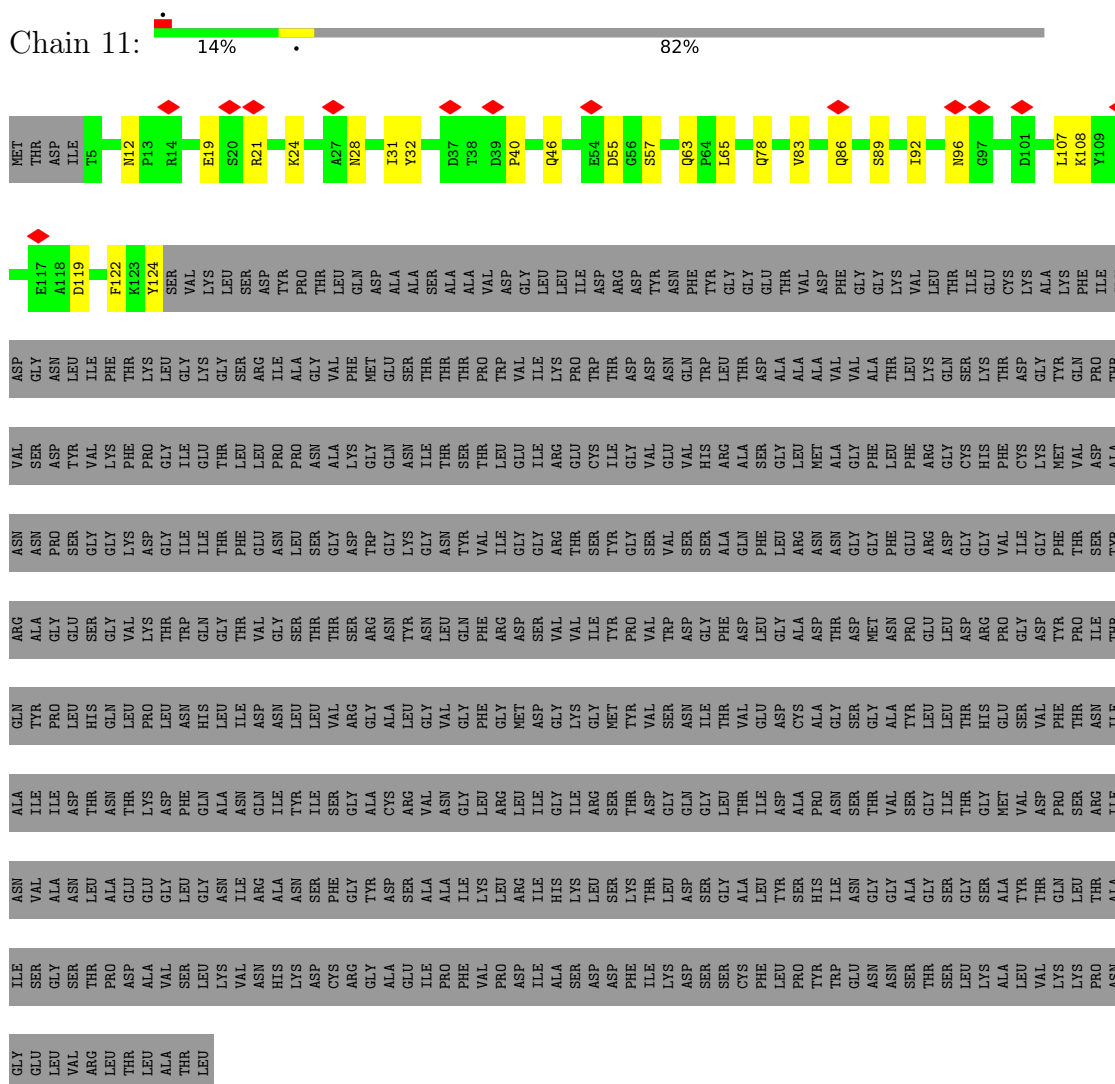
Chain 21:  12% 6% 82%



● Molecule 4: Tail spike protein



- Molecule 4: Tail spike protein

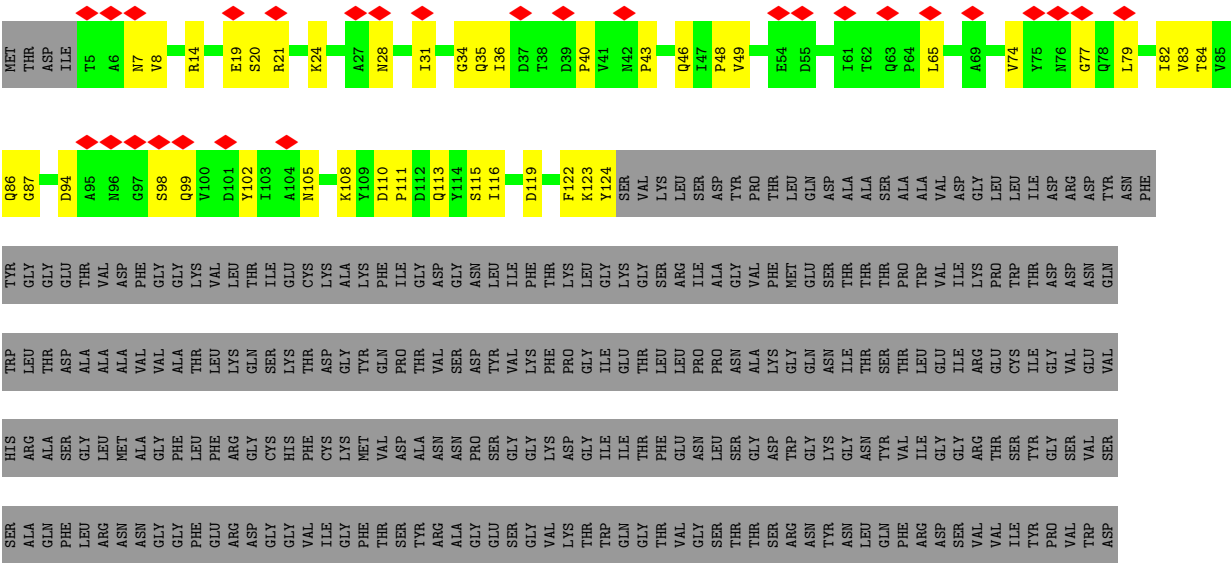


- Molecule 4: Tail spike protein





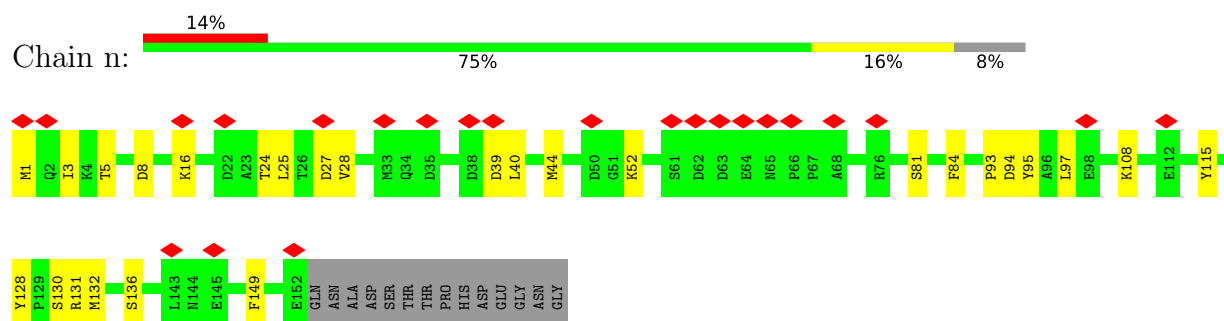
● Molecule 4: Tail spike protein



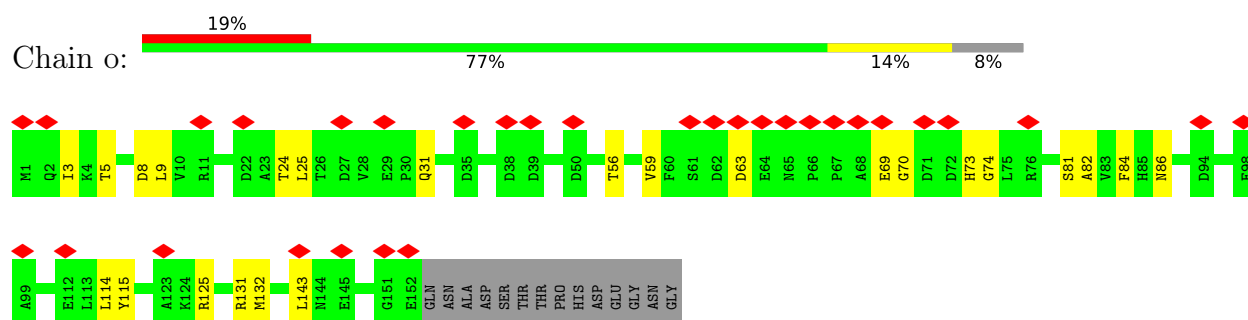
Chain 15: 15% 82%



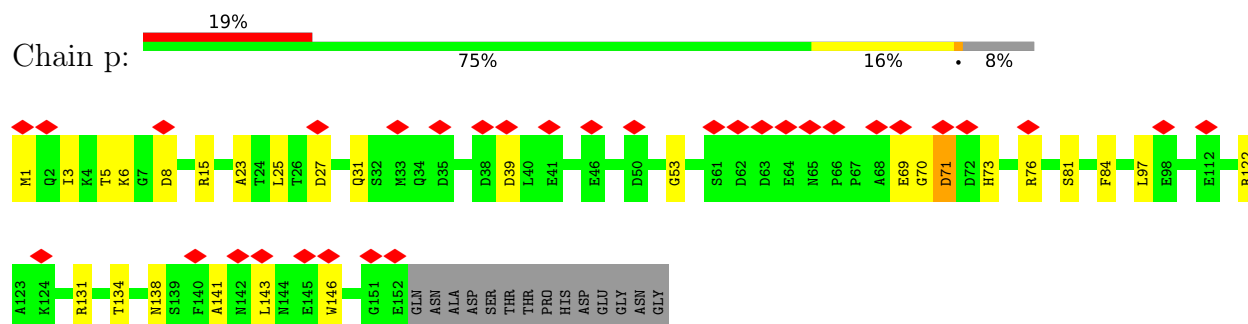
• Molecule 5: Peptidoglycan hydrolase gp4



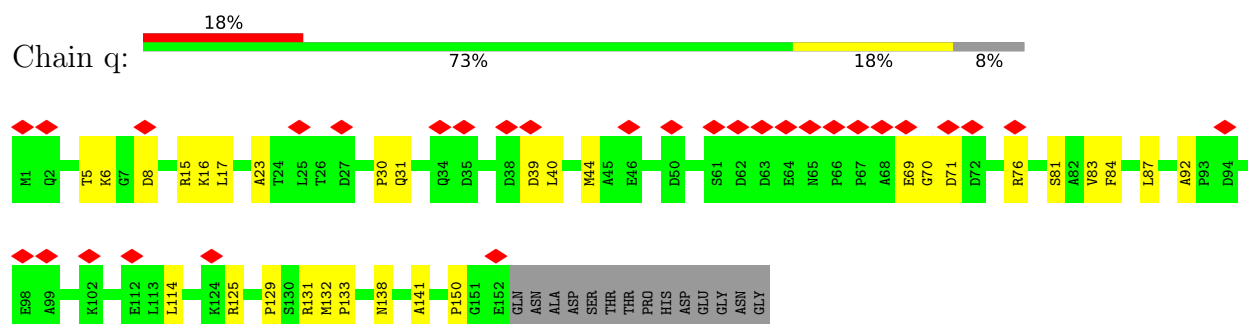
• Molecule 5: Peptidoglycan hydrolase gp4



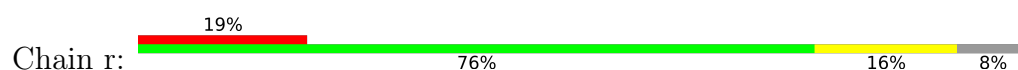
• Molecule 5: Peptidoglycan hydrolase gp4

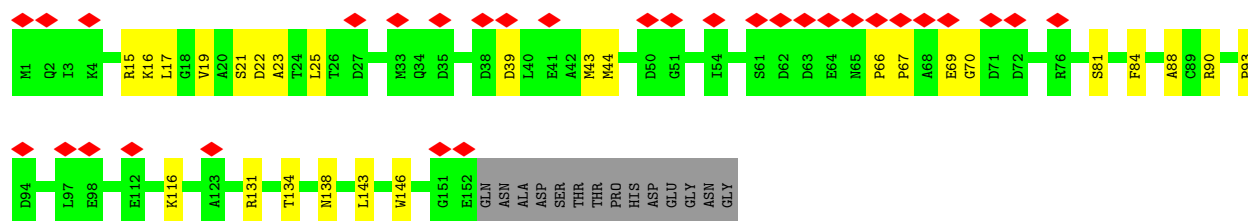


• Molecule 5: Peptidoglycan hydrolase gp4

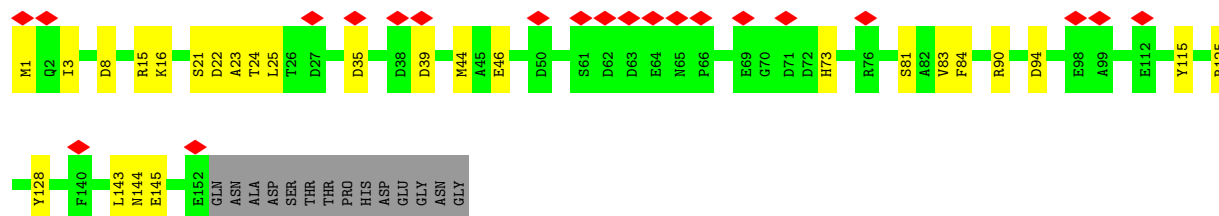
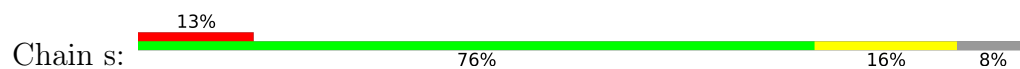


• Molecule 5: Peptidoglycan hydrolase gp4

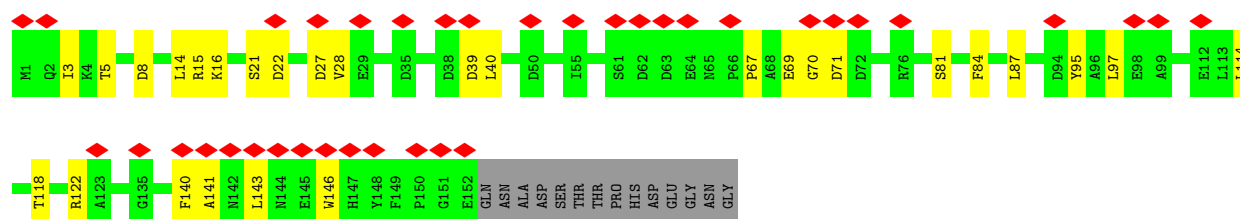
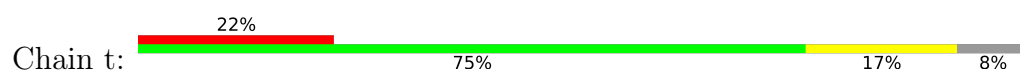




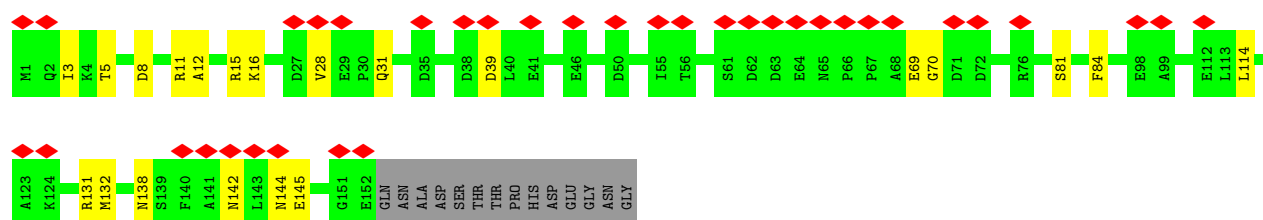
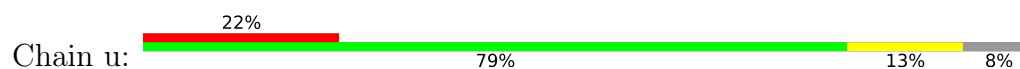
• Molecule 5: Peptidoglycan hydrolase gp4



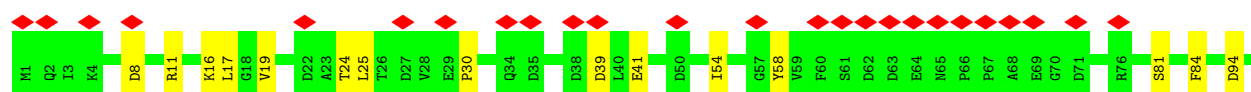
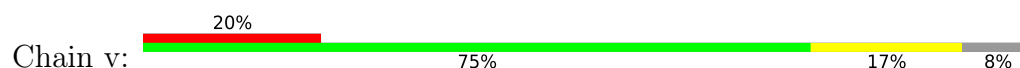
• Molecule 5: Peptidoglycan hydrolase gp4



• Molecule 5: Peptidoglycan hydrolase gp4



• Molecule 5: Peptidoglycan hydrolase gp4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18053	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.218	Depositor
Minimum map value	-14.936	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.15	0/4512	0.30	0/6117
1	b	0.14	0/4512	0.29	0/6117
1	c	0.15	0/4512	0.31	0/6117
1	d	0.13	0/4512	0.28	0/6117
1	e	0.13	0/4512	0.32	2/6117 (0.0%)
1	f	0.13	0/4512	0.29	0/6117
1	g	0.16	0/4512	0.31	0/6117
1	h	0.14	0/4512	0.29	0/6117
1	i	0.13	0/4512	0.29	0/6117
1	j	0.14	0/4512	0.31	0/6117
1	k	0.13	0/4512	0.29	0/6117
1	l	0.15	0/4512	0.31	0/6117
2	A	0.17	0/3335	0.37	1/4535 (0.0%)
2	B	0.19	0/3277	0.35	0/4456
2	C	0.17	0/3335	0.37	1/4535 (0.0%)
2	D	0.18	0/3277	0.33	0/4456
2	E	0.15	0/3335	0.32	0/4535
2	F	0.18	0/3277	0.35	0/4456
2	G	0.16	0/3335	0.35	0/4535
2	H	0.19	0/3277	0.36	0/4456
2	I	0.17	0/3335	0.32	0/4535
2	J	0.19	0/3277	0.34	0/4456
3	1	0.16	0/3764	0.36	0/5097
3	2	0.15	0/3764	0.33	0/5097
3	3	0.15	0/3764	0.36	0/5097
3	4	0.14	0/3764	0.32	0/5097
3	5	0.14	0/3764	0.34	0/5097
3	6	0.14	0/3764	0.34	0/5097
4	10	0.17	0/953	0.42	0/1299
4	11	0.18	0/953	0.34	0/1299
4	12	0.16	0/953	0.37	0/1299
4	13	0.14	0/953	0.35	0/1299
4	14	0.16	0/953	0.34	0/1299
4	15	0.15	0/953	0.35	0/1299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	16	0.15	0/953	0.35	0/1299
4	17	0.16	0/953	0.32	0/1299
4	18	0.17	0/953	0.36	0/1299
4	19	0.16	0/953	0.33	0/1299
4	20	0.19	0/953	0.38	0/1299
4	21	0.15	0/953	0.35	0/1299
4	22	0.15	0/953	0.37	0/1299
4	23	0.18	0/953	0.32	0/1299
4	24	0.16	0/953	0.35	0/1299
4	7	0.16	0/953	0.34	0/1299
4	8	0.19	0/953	0.37	0/1299
4	9	0.14	0/953	0.33	0/1299
5	m	0.15	0/1191	0.32	0/1614
5	n	0.22	0/1191	0.48	2/1614 (0.1%)
5	o	0.19	0/1191	0.37	0/1614
5	p	0.19	0/1191	0.36	0/1614
5	q	0.16	0/1191	0.33	0/1614
5	r	0.15	0/1191	0.31	0/1614
5	s	0.19	0/1191	0.34	0/1614
5	t	0.14	0/1191	0.29	0/1614
5	u	0.17	0/1191	0.34	0/1614
5	v	0.17	0/1191	0.35	0/1614
5	x	0.17	0/1191	0.34	0/1614
5	y	0.16	0/1191	0.34	0/1614
All	All	0.16	0/141234	0.33	6/191691 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
1	c	0	1
1	j	0	1
1	l	0	1
3	3	0	1
3	5	0	1
4	18	0	1
5	p	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	n	93	PRO	CA-N-CD	-10.69	97.03	112.00
2	C	336	ASP	CB-CA-C	-5.90	109.75	116.54
2	A	336	ASP	CB-CA-C	-5.64	110.05	116.54
1	e	208	VAL	CA-C-N	-5.36	109.66	122.74
1	e	208	VAL	C-N-CA	-5.36	109.66	122.74

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	287	GLU	Peptide
1	a	328	ARG	Sidechain
1	c	45	LEU	Peptide
1	j	37	ARG	Sidechain
1	l	72	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	4417	0	4295	93	0
1	b	4417	0	4295	80	0
1	c	4417	0	4295	76	0
1	d	4417	0	4295	78	0
1	e	4417	0	4295	71	0
1	f	4417	0	4295	79	0
1	g	4417	0	4295	97	0
1	h	4417	0	4295	83	0
1	i	4417	0	4295	65	0
1	j	4417	0	4295	96	0
1	k	4417	0	4295	86	0
1	l	4417	0	4295	102	0
2	A	3277	0	3247	80	0
2	B	3219	0	3185	81	0
2	C	3277	0	3247	86	0
2	D	3219	0	3188	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3277	0	3247	60	0
2	F	3219	0	3188	80	0
2	G	3277	0	3247	64	0
2	H	3219	0	3188	69	0
2	I	3277	0	3247	60	0
2	J	3219	0	3188	78	0
3	1	3683	0	3590	100	0
3	2	3683	0	3590	91	0
3	3	3683	0	3590	88	0
3	4	3683	0	3590	82	0
3	5	3683	0	3590	86	0
3	6	3683	0	3590	79	0
4	10	934	0	925	19	0
4	11	934	0	925	23	0
4	12	934	0	925	24	0
4	13	934	0	925	32	0
4	14	934	0	925	18	0
4	15	934	0	925	19	0
4	16	934	0	925	29	0
4	17	934	0	925	26	0
4	18	934	0	925	24	0
4	19	934	0	925	32	0
4	20	934	0	925	23	0
4	21	934	0	925	31	0
4	22	934	0	925	25	0
4	23	934	0	925	28	0
4	24	934	0	925	23	0
4	7	934	0	925	26	0
4	8	934	0	925	33	0
4	9	934	0	925	23	0
5	m	1166	0	1133	16	0
5	n	1166	0	1133	20	0
5	o	1166	0	1133	18	0
5	p	1166	0	1133	20	0
5	q	1166	0	1133	27	0
5	r	1166	0	1133	19	0
5	s	1166	0	1133	20	0
5	t	1166	0	1133	26	0
5	u	1166	0	1133	17	0
5	v	1166	0	1133	25	0
5	x	1166	0	1133	21	0
5	y	1166	0	1133	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	138386	0	135498	2436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 2436 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:20:105:ASN:HD22	4:20:108:LYS:HG2	1.35	0.91
2:I:70:LEU:HB2	2:J:95:ARG:HD2	1.52	0.91
4:19:31:ILE:HB	4:19:65:LEU:HB2	1.57	0.85
2:I:309:THR:HG23	2:I:310:PRO:HD3	1.59	0.85
2:A:70:LEU:HD12	2:B:95:ARG:HH22	1.42	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	538/725 (74%)	515 (96%)	23 (4%)	0	100	100
1	b	538/725 (74%)	508 (94%)	28 (5%)	2 (0%)	30	62
1	c	538/725 (74%)	509 (95%)	29 (5%)	0	100	100
1	d	538/725 (74%)	516 (96%)	21 (4%)	1 (0%)	43	73
1	e	538/725 (74%)	507 (94%)	30 (6%)	1 (0%)	43	73
1	f	538/725 (74%)	512 (95%)	25 (5%)	1 (0%)	43	73
1	g	538/725 (74%)	513 (95%)	25 (5%)	0	100	100
1	h	538/725 (74%)	520 (97%)	18 (3%)	0	100	100
1	i	538/725 (74%)	516 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	538/725 (74%)	514 (96%)	23 (4%)	1 (0%)	43	73
1	k	538/725 (74%)	517 (96%)	20 (4%)	1 (0%)	43	73
1	l	538/725 (74%)	508 (94%)	28 (5%)	2 (0%)	30	62
2	A	427/430 (99%)	400 (94%)	26 (6%)	1 (0%)	43	73
2	B	419/430 (97%)	403 (96%)	14 (3%)	2 (0%)	24	59
2	C	427/430 (99%)	397 (93%)	29 (7%)	1 (0%)	43	73
2	D	419/430 (97%)	405 (97%)	12 (3%)	2 (0%)	24	59
2	E	427/430 (99%)	405 (95%)	22 (5%)	0	100	100
2	F	419/430 (97%)	397 (95%)	20 (5%)	2 (0%)	24	59
2	G	427/430 (99%)	401 (94%)	26 (6%)	0	100	100
2	H	419/430 (97%)	404 (96%)	13 (3%)	2 (0%)	24	59
2	I	427/430 (99%)	399 (93%)	28 (7%)	0	100	100
2	J	419/430 (97%)	403 (96%)	14 (3%)	2 (0%)	24	59
3	1	469/472 (99%)	439 (94%)	29 (6%)	1 (0%)	43	73
3	2	469/472 (99%)	434 (92%)	35 (8%)	0	100	100
3	3	469/472 (99%)	436 (93%)	33 (7%)	0	100	100
3	4	469/472 (99%)	435 (93%)	34 (7%)	0	100	100
3	5	469/472 (99%)	433 (92%)	36 (8%)	0	100	100
3	6	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
4	10	118/667 (18%)	115 (98%)	3 (2%)	0	100	100
4	11	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
4	12	118/667 (18%)	116 (98%)	2 (2%)	0	100	100
4	13	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	14	118/667 (18%)	115 (98%)	3 (2%)	0	100	100
4	15	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
4	16	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	17	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	18	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	19	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
4	20	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
4	21	118/667 (18%)	113 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	22	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
4	23	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	24	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	7	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
4	8	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
4	9	118/667 (18%)	113 (96%)	5 (4%)	0	100	100
5	m	150/166 (90%)	144 (96%)	6 (4%)	0	100	100
5	n	150/166 (90%)	144 (96%)	6 (4%)	0	100	100
5	o	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
5	p	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
5	q	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
5	r	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
5	s	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
5	t	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
5	u	150/166 (90%)	143 (95%)	6 (4%)	1 (1%)	18	52
5	v	150/166 (90%)	144 (96%)	6 (4%)	0	100	100
5	x	150/166 (90%)	143 (95%)	7 (5%)	0	100	100
5	y	150/166 (90%)	141 (94%)	9 (6%)	0	100	100
All	All	17424/29830 (58%)	16558 (95%)	843 (5%)	23 (0%)	49	79

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	214	GLN
1	l	242	GLU
2	J	283	GLN
1	d	49	THR
1	f	210	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	480/630 (76%)	476 (99%)	4 (1%)	73	82
1	b	480/630 (76%)	479 (100%)	1 (0%)	87	89
1	c	480/630 (76%)	476 (99%)	4 (1%)	73	82
1	d	480/630 (76%)	479 (100%)	1 (0%)	87	89
1	e	480/630 (76%)	478 (100%)	2 (0%)	84	86
1	f	480/630 (76%)	478 (100%)	2 (0%)	84	86
1	g	480/630 (76%)	477 (99%)	3 (1%)	78	84
1	h	480/630 (76%)	479 (100%)	1 (0%)	87	89
1	i	480/630 (76%)	477 (99%)	3 (1%)	78	84
1	j	480/630 (76%)	479 (100%)	1 (0%)	87	89
1	k	480/630 (76%)	479 (100%)	1 (0%)	87	89
1	l	480/630 (76%)	478 (100%)	2 (0%)	84	86
2	A	351/352 (100%)	350 (100%)	1 (0%)	86	88
2	B	345/352 (98%)	338 (98%)	7 (2%)	48	72
2	C	351/352 (100%)	350 (100%)	1 (0%)	86	88
2	D	345/352 (98%)	338 (98%)	7 (2%)	48	72
2	E	351/352 (100%)	348 (99%)	3 (1%)	70	81
2	F	345/352 (98%)	340 (99%)	5 (1%)	59	77
2	G	351/352 (100%)	349 (99%)	2 (1%)	78	84
2	H	345/352 (98%)	342 (99%)	3 (1%)	70	81
2	I	351/352 (100%)	351 (100%)	0	100	100
2	J	345/352 (98%)	342 (99%)	3 (1%)	70	81
3	1	394/395 (100%)	388 (98%)	6 (2%)	57	76
3	2	394/395 (100%)	392 (100%)	2 (0%)	81	85
3	3	394/395 (100%)	391 (99%)	3 (1%)	73	82
3	4	394/395 (100%)	391 (99%)	3 (1%)	73	82
3	5	394/395 (100%)	392 (100%)	2 (0%)	81	85
3	6	394/395 (100%)	388 (98%)	6 (2%)	57	76
4	10	103/548 (19%)	103 (100%)	0	100	100
4	11	103/548 (19%)	101 (98%)	2 (2%)	50	73
4	12	103/548 (19%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	13	103/548 (19%)	101 (98%)	2 (2%)	50	73
4	14	103/548 (19%)	101 (98%)	2 (2%)	50	73
4	15	103/548 (19%)	103 (100%)	0	100	100
4	16	103/548 (19%)	103 (100%)	0	100	100
4	17	103/548 (19%)	102 (99%)	1 (1%)	68	80
4	18	103/548 (19%)	101 (98%)	2 (2%)	50	73
4	19	103/548 (19%)	102 (99%)	1 (1%)	68	80
4	20	103/548 (19%)	102 (99%)	1 (1%)	68	80
4	21	103/548 (19%)	101 (98%)	2 (2%)	50	73
4	22	103/548 (19%)	103 (100%)	0	100	100
4	23	103/548 (19%)	102 (99%)	1 (1%)	68	80
4	24	103/548 (19%)	102 (99%)	1 (1%)	68	80
4	7	103/548 (19%)	103 (100%)	0	100	100
4	8	103/548 (19%)	100 (97%)	3 (3%)	37	67
4	9	103/548 (19%)	102 (99%)	1 (1%)	68	80
5	m	120/131 (92%)	120 (100%)	0	100	100
5	n	120/131 (92%)	118 (98%)	2 (2%)	53	75
5	o	120/131 (92%)	120 (100%)	0	100	100
5	p	120/131 (92%)	118 (98%)	2 (2%)	53	75
5	q	120/131 (92%)	120 (100%)	0	100	100
5	r	120/131 (92%)	120 (100%)	0	100	100
5	s	120/131 (92%)	119 (99%)	1 (1%)	73	82
5	t	120/131 (92%)	120 (100%)	0	100	100
5	u	120/131 (92%)	120 (100%)	0	100	100
5	v	120/131 (92%)	119 (99%)	1 (1%)	73	82
5	x	120/131 (92%)	118 (98%)	2 (2%)	53	75
5	y	120/131 (92%)	118 (98%)	2 (2%)	53	75
All	All	14898/24886 (60%)	14790 (99%)	108 (1%)	73	83

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	37	LEU

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Mol	Chain	Res	Type
3	5	359	VAL
5	y	26	THR
3	1	189	ILE
3	3	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	234	GLN
4	22	45	ASN
3	3	267	GLN
3	5	370	GLN
4	19	88	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

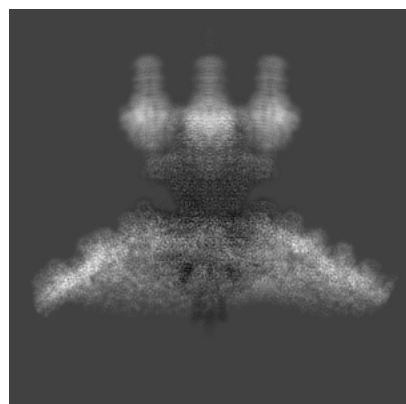
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41791. These allow visual inspection of the internal detail of the map and identification of artifacts.

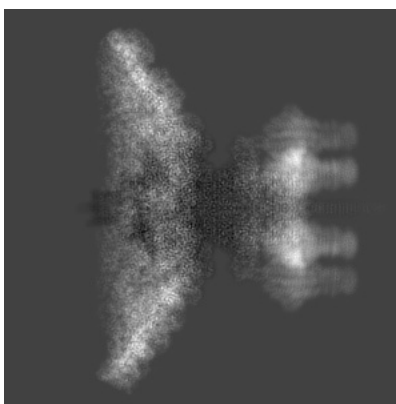
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

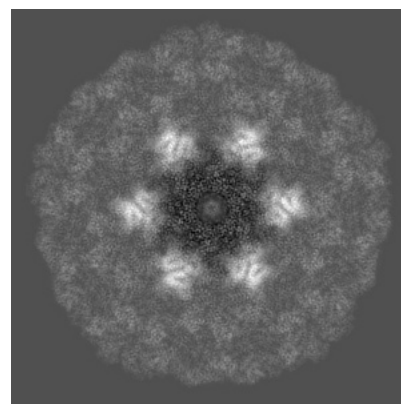
6.1.1 Primary map



X

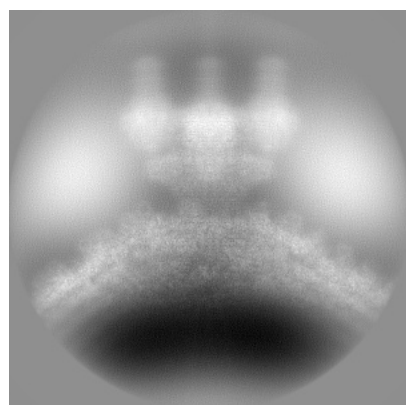


Y

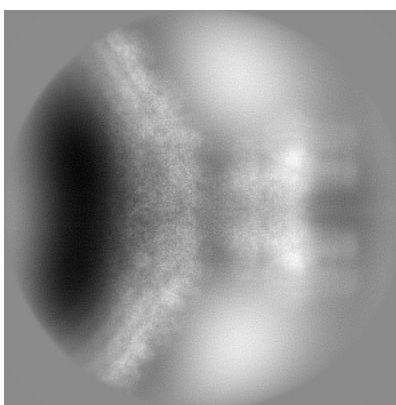


Z

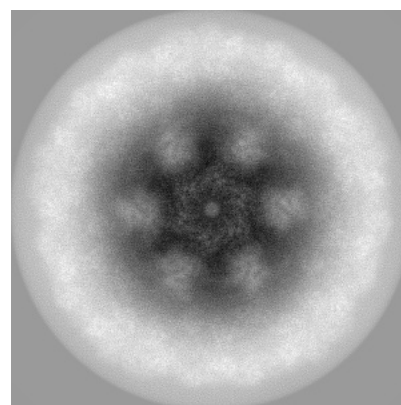
6.1.2 Raw map



X



Y

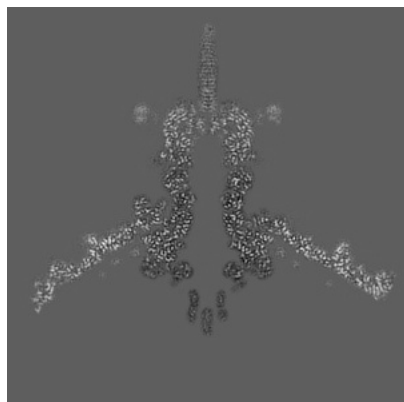


Z

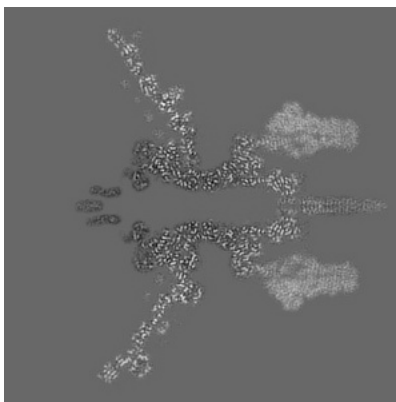
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

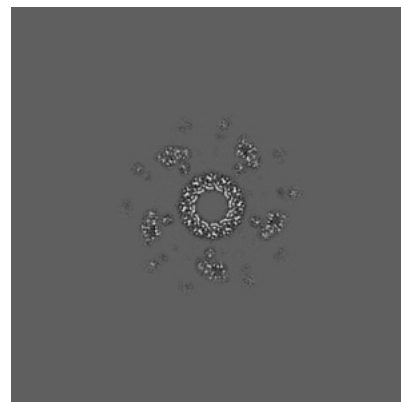
6.2.1 Primary map



X Index: 220

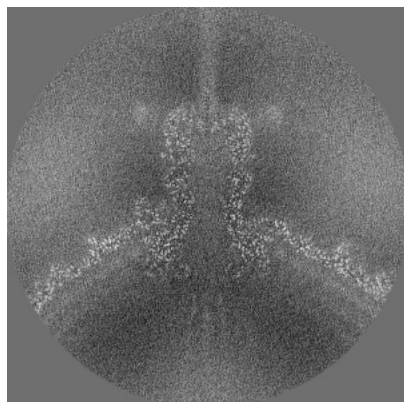


Y Index: 220

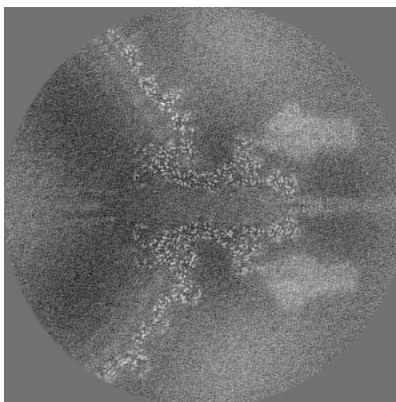


Z Index: 220

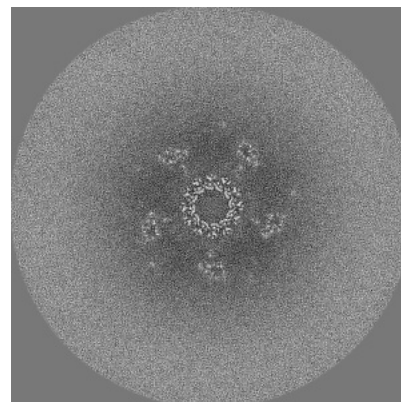
6.2.2 Raw map



X Index: 220



Y Index: 220

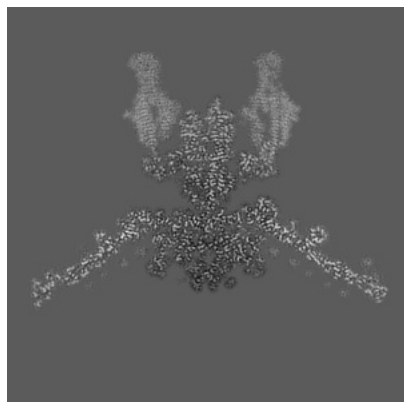


Z Index: 220

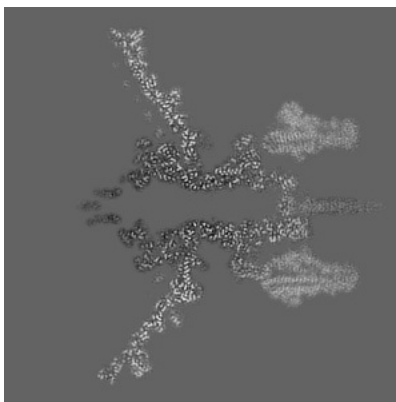
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

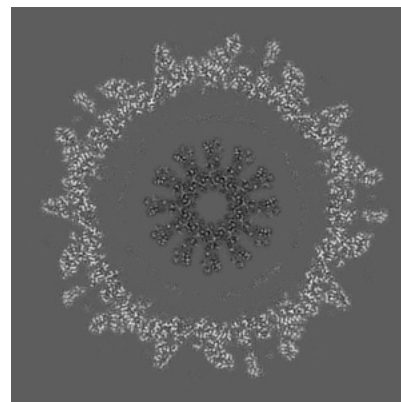
6.3.1 Primary map



X Index: 254

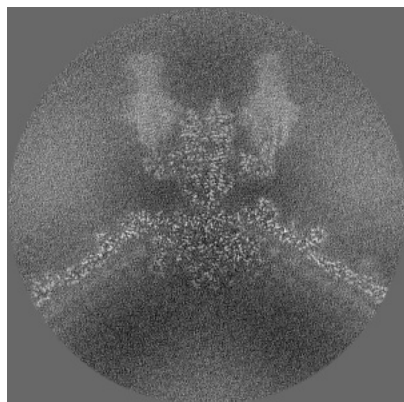


Y Index: 215

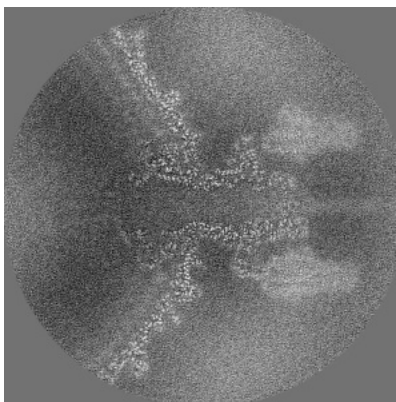


Z Index: 153

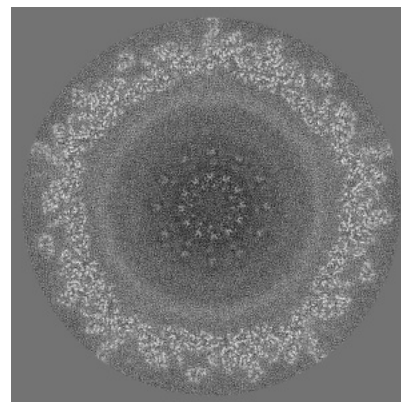
6.3.2 Raw map



X Index: 254



Y Index: 214

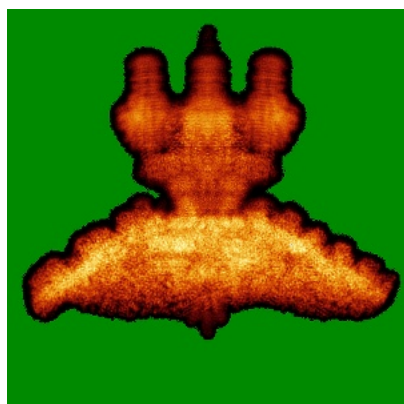


Z Index: 144

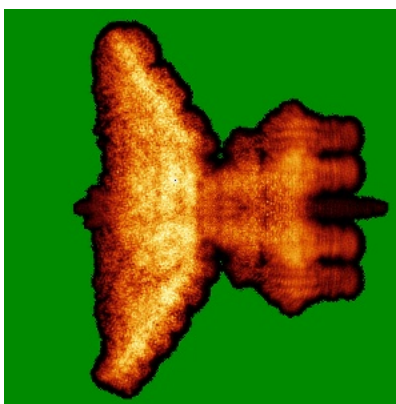
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

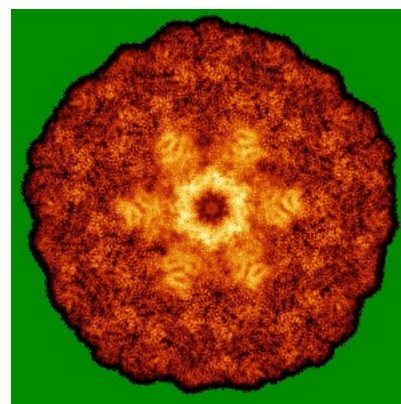
6.4.1 Primary map



X

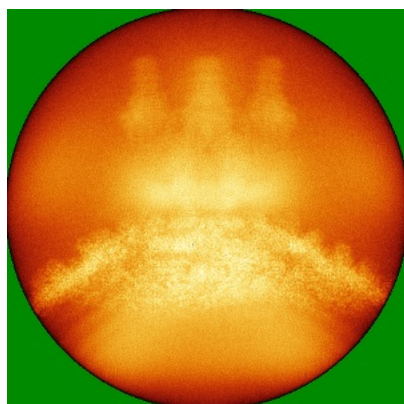


Y

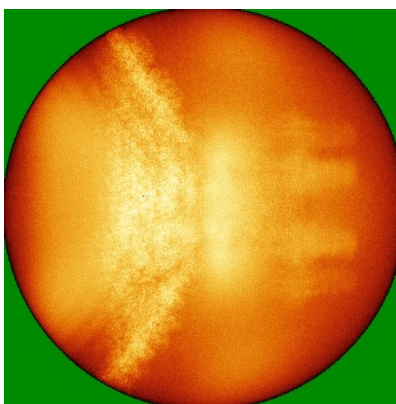


Z

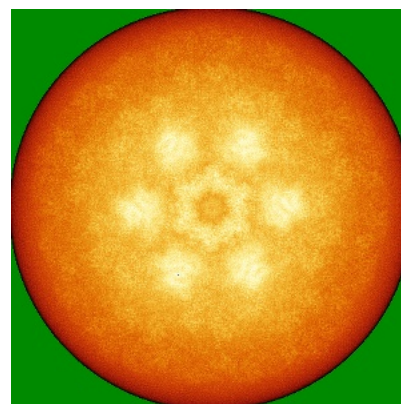
6.4.2 Raw map



X



Y

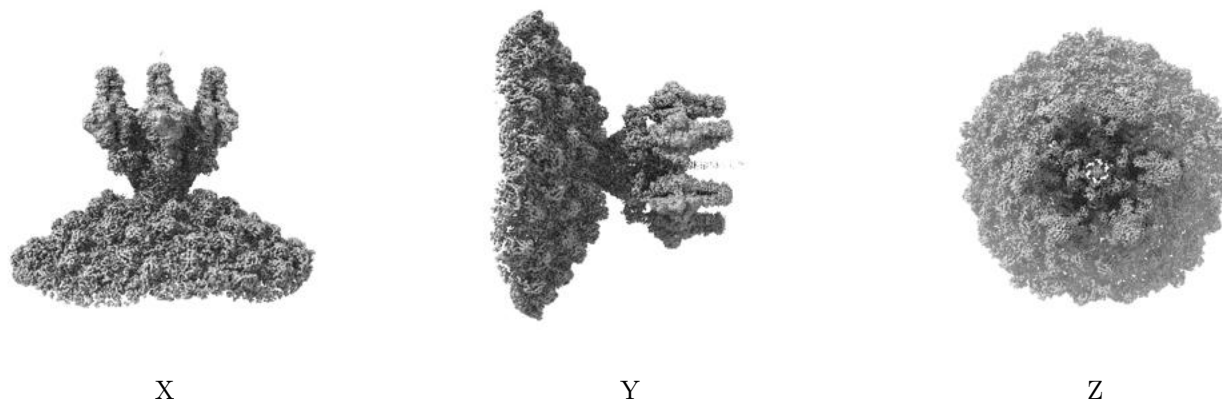


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

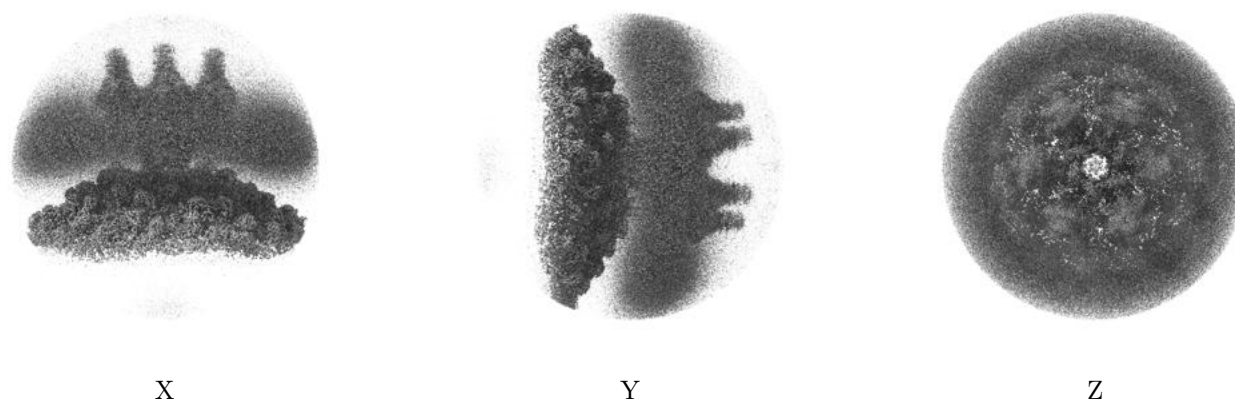
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

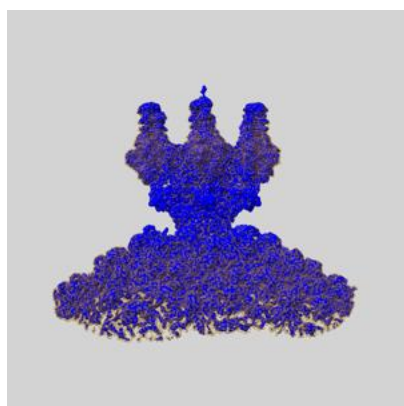
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

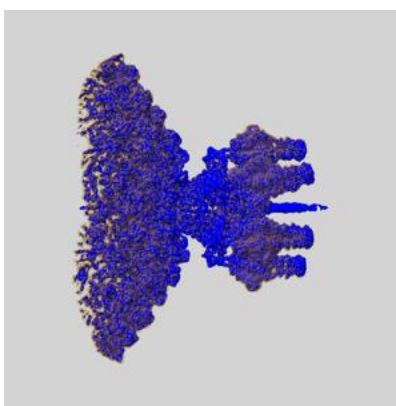
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

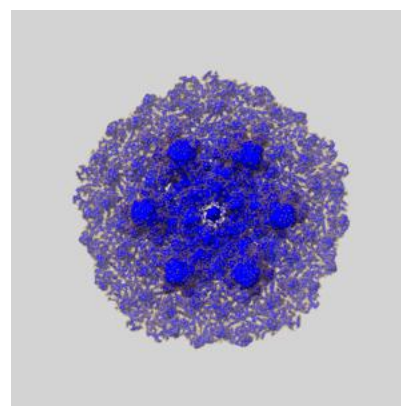
6.6.1 emd_41791_msk_1.map [i](#)



X



Y

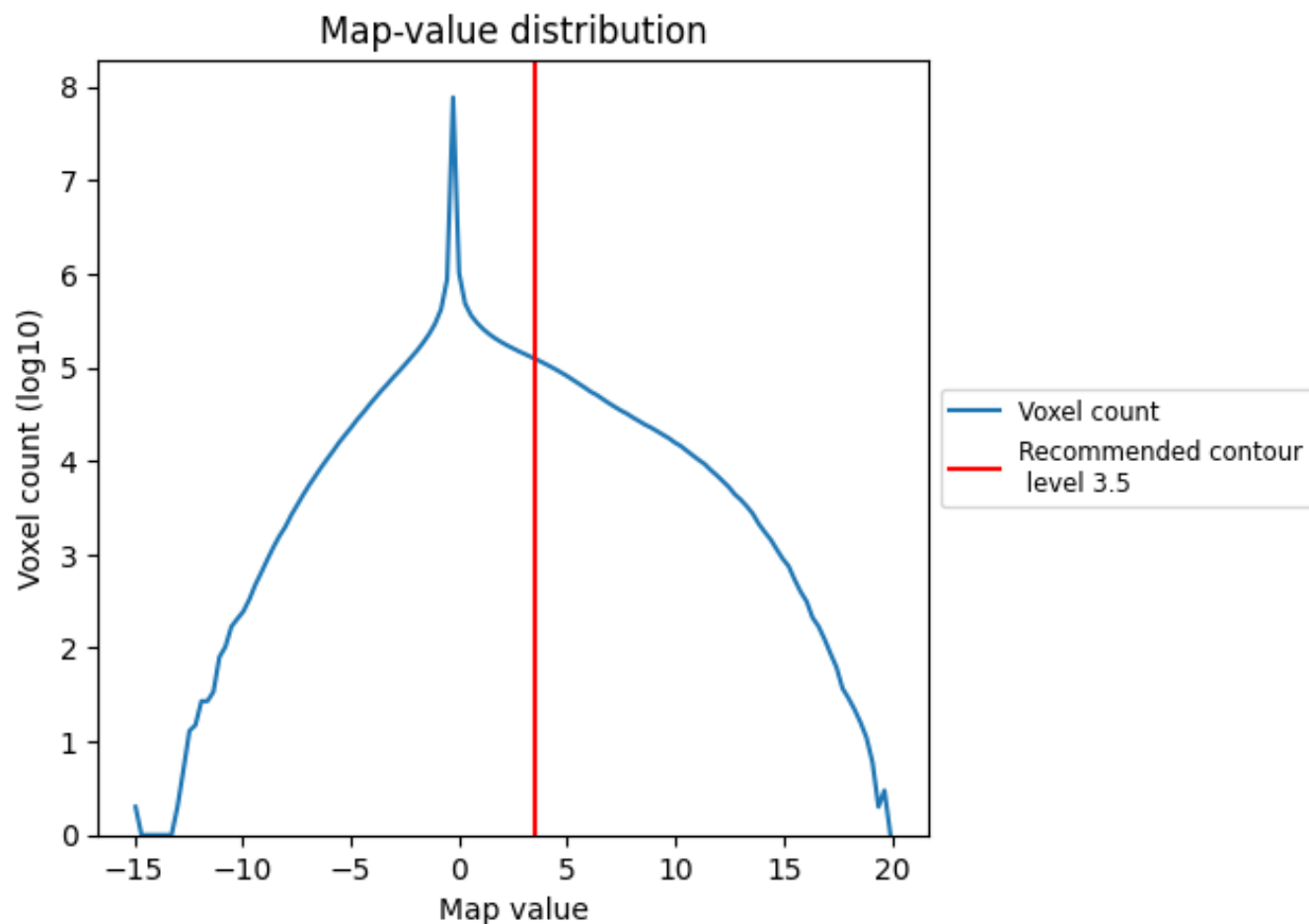


Z

7 Map analysis [i](#)

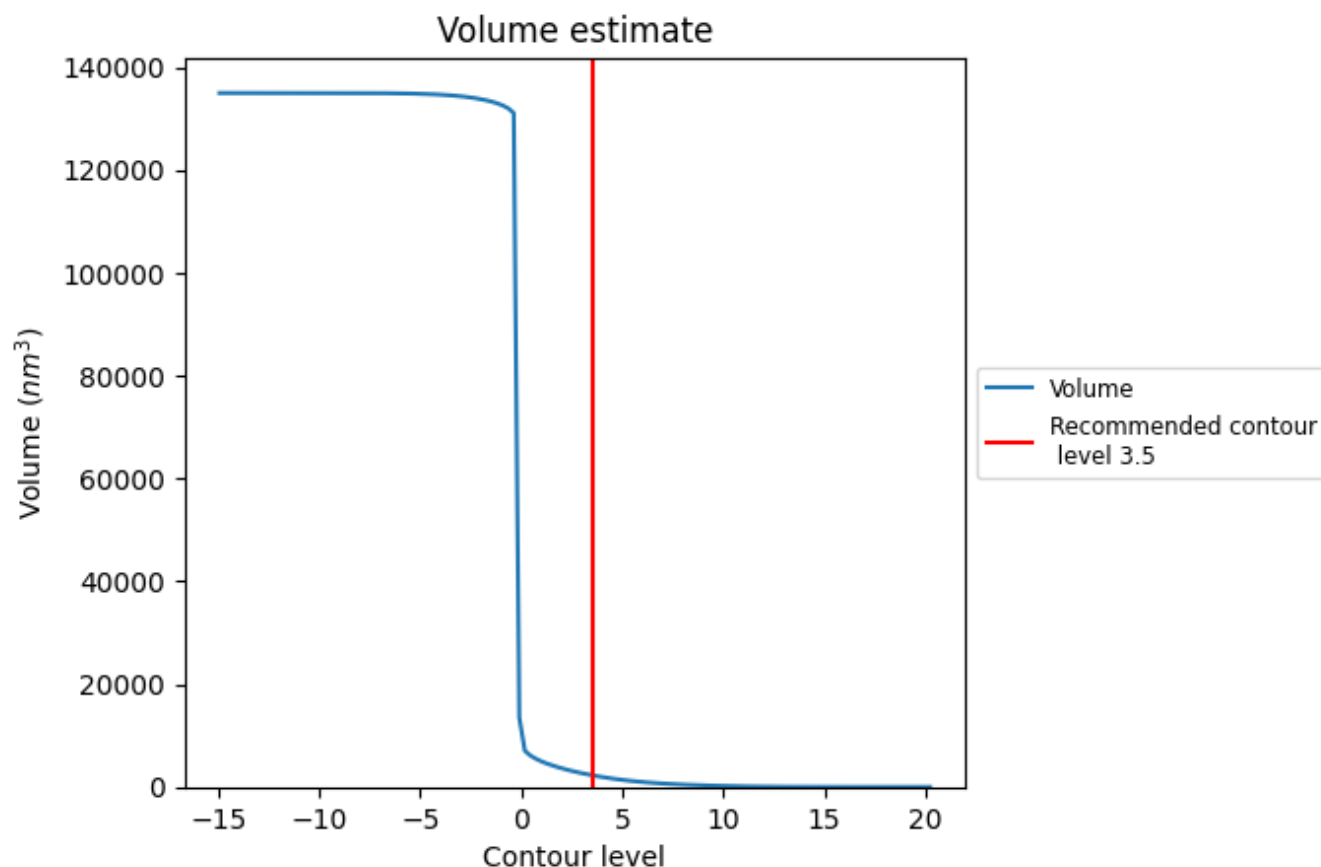
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

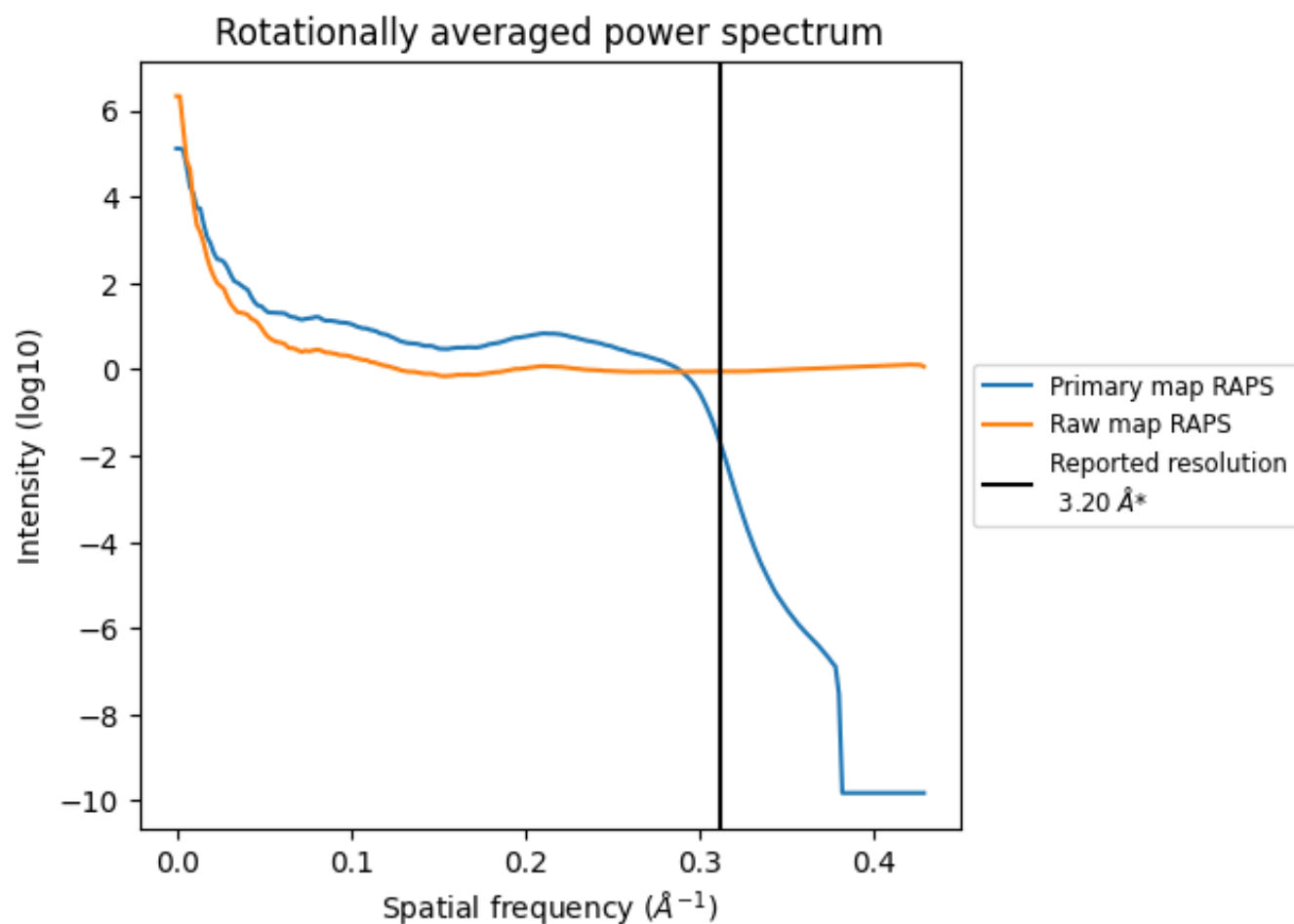
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2274 nm^3 ; this corresponds to an approximate mass of 2054 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

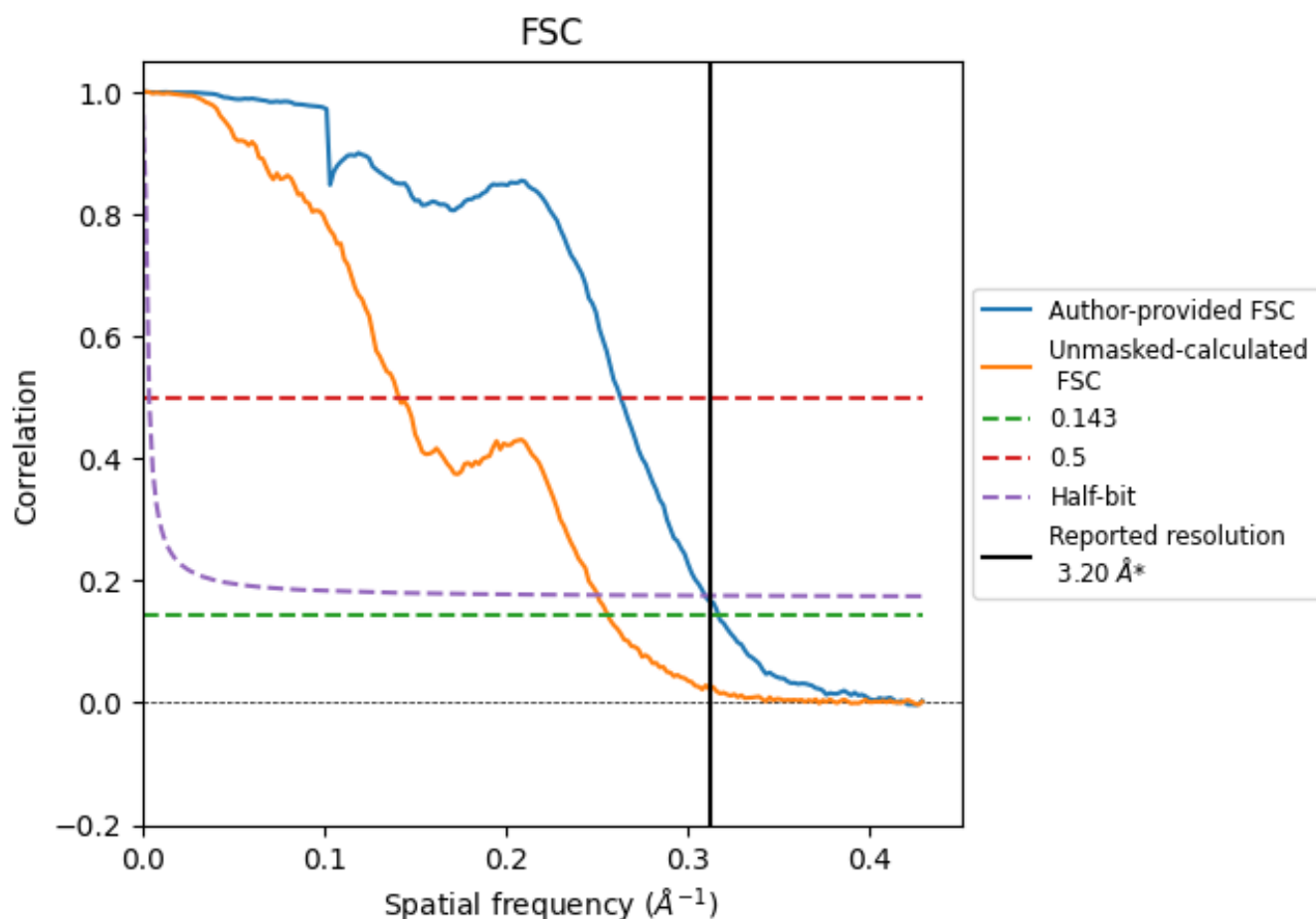


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

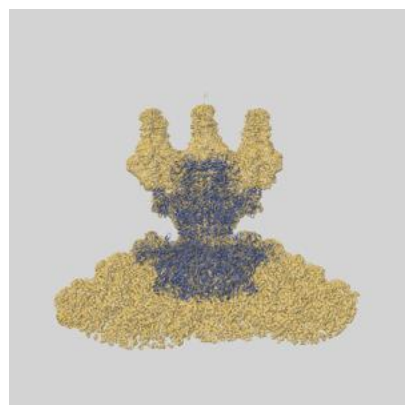
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.80	3.23
Unmasked-calculated*	3.90	7.09	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.2 by more than 10 %

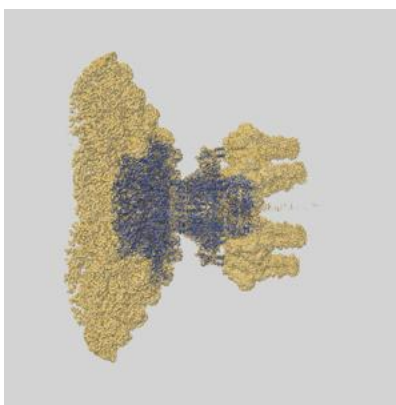
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41791 and PDB model 8U10. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

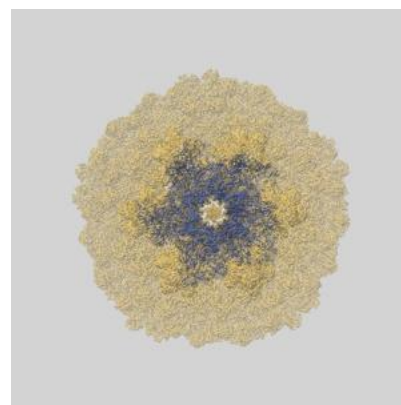
9.1 Map-model overlay [i](#)



X



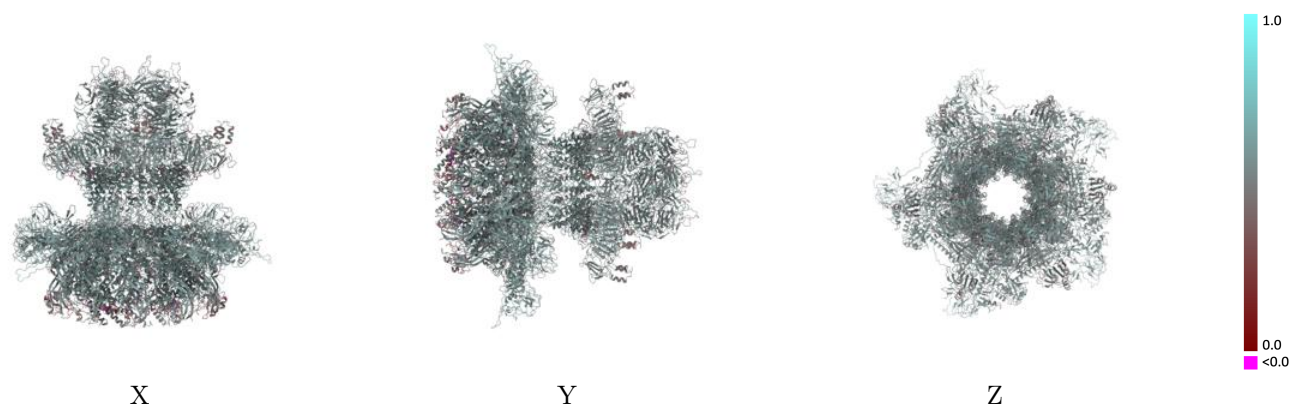
Y



Z

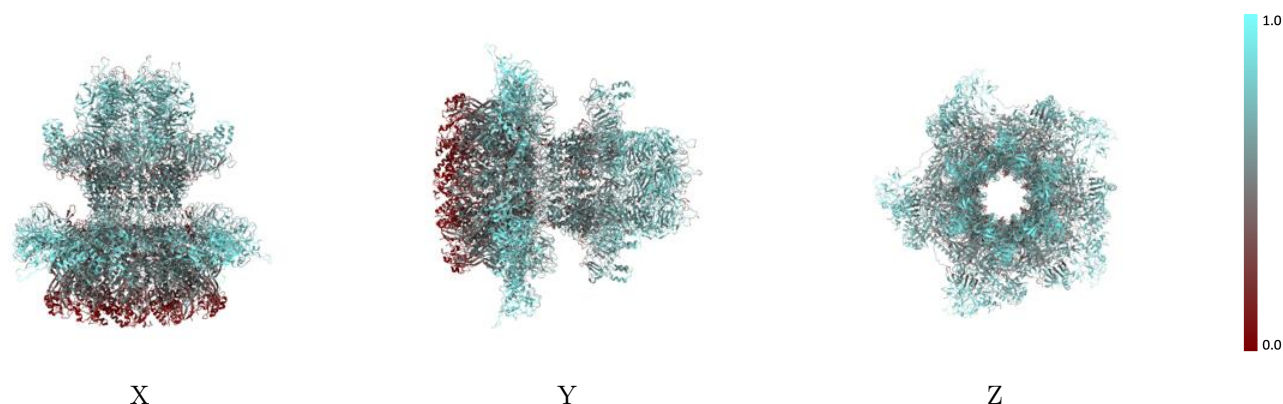
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



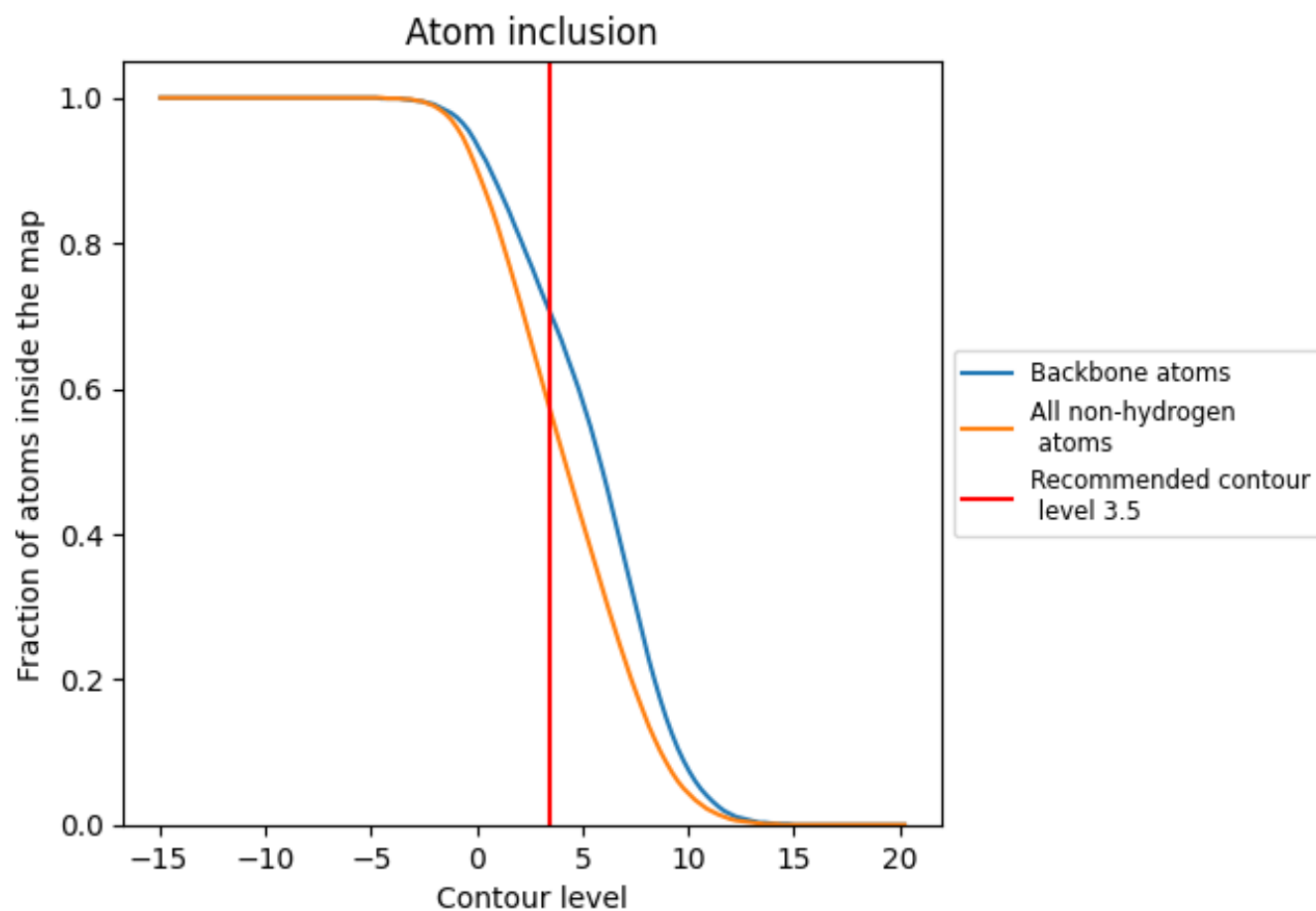
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.5280
1	 0.6850	 0.5340
10	 0.6090	 0.4950
11	 0.6270	 0.5300
12	 0.6530	 0.5280
13	 0.5990	 0.4930
14	 0.6130	 0.5170
15	 0.6640	 0.5230
16	 0.5900	 0.4980
17	 0.6290	 0.5210
18	 0.6760	 0.5380
19	 0.5950	 0.4980
2	 0.6930	 0.5300
20	 0.6280	 0.5110
21	 0.6570	 0.5250
22	 0.6130	 0.4930
23	 0.6510	 0.5200
24	 0.6640	 0.5290
3	 0.6780	 0.5310
4	 0.6950	 0.5310
5	 0.6920	 0.5300
6	 0.6980	 0.5340
7	 0.5940	 0.4930
8	 0.6520	 0.5240
9	 0.6670	 0.5300
A	 0.6410	 0.5370
B	 0.7540	 0.5510
C	 0.6450	 0.5370
D	 0.7490	 0.5580
E	 0.6590	 0.5500
F	 0.7250	 0.5420
G	 0.6440	 0.5460
H	 0.7490	 0.5520
I	 0.6590	 0.5480
J	 0.7180	 0.5410



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Chain	Atom inclusion	Q-score
a	 0.4240	 0.5190
b	 0.4250	 0.5170
c	 0.4230	 0.5220
d	 0.4360	 0.5230
e	 0.4210	 0.5190
f	 0.4140	 0.5140
g	 0.4060	 0.5110
h	 0.4090	 0.5160
i	 0.4220	 0.5190
j	 0.4240	 0.5180
k	 0.4330	 0.5250
l	 0.4120	 0.5200
m	 0.5580	 0.5340
n	 0.5980	 0.5450
o	 0.5410	 0.5130
p	 0.5540	 0.5380
q	 0.5640	 0.5380
r	 0.5560	 0.5310
s	 0.5790	 0.5500
t	 0.5310	 0.5400
u	 0.5420	 0.5220
v	 0.5350	 0.5260
x	 0.5790	 0.5370
y	 0.5550	 0.5400